

SEARCH REQUEST FORM

273007

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SEP 22 2008

STIC

Requester's Full Name: Cecilia Joise Examiner: _____ Date: 9-19-08
 Art Unit: 1624 Phone Number: 2-9931 Serial Number: 10590786
 Location (Bldg/Room#): REM 5428 (Mailbox #): 5018 Results Format Preferred (circle): PAPER DIS

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: See Bib Data Sheet
 Inventors (please provide full names): _____

Earliest Priority Date: _____

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include selected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

See claims attached. Please do structure search and inventor name(s) search. Display results to show identification of source, and RN #, compound name & structure of identified compounds. Search Compounds of Formula I as amended. See previous search.

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Please call with any questions

STAFF USE ONLY

| Searcher: | Type of Search | Vendors and eqpt where applicable |
|------------------------------|-----------------|-----------------------------------------------------------|
| Searcher Phone #: | HA Sequence (#) | STN _____ Dialog _____ |
| Searcher Location: | AA Sequence (#) | Quartel/Orbit _____ Lexis/Nexis _____ |
| Date Searcher Picked Up: | Structure (#) | Westlaw _____ W.W./Intertec _____ |
| Date Completed: | Biological | In-house sequence systems _____ |
| Searcher Prep & Review Time: | Litigation | Commercial _____ Oligomer _____ Source/Leads _____ |
| Online Time: | Patent | Interference _____ SPDI _____ Bioscience/Trademarks _____ |
| | Other | Other (specify) _____ |

STRUCTURE SEARCH

=> fil reg; d stat que 15; fil zcap1; d que nos 16; d ibib abs hitstr 16 1-11; fil hom

FILE 'REGISTRY' ENTERED AT 12:36:44 ON 22 SEP 2008

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 SEP 2008 HIGHEST RN 1051326-19-2

DICTIONARY FILE UPDATES: 21 SEP 2008 HIGHEST RN 1051326-19-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

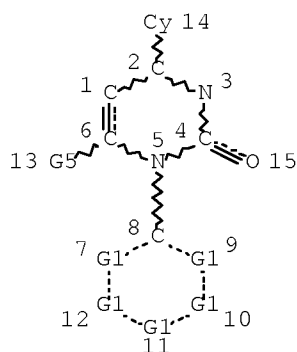
TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

L1 STR



VAR G1=C/N

VAR G5=C/NH2

NODE ATTRIBUTES:

CONNECT IS E3 RC AT 1

CONNECT IS E3 RC AT 3

DEFAULT MLEVEL IS ATOM

GGCAT IS UNS AT 14

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

L5 397 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 94555 ITERATIONS

397 ANSWERS

SEARCH TIME: 00.00.04

FILE 'ZCAPLUS' ENTERED AT 12:36:45 ON 22 SEP 2008

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FILE COVERS 1907 - 22 Sep 2008 VOL 149 ISS 13

FILE LAST UPDATED: 21 Sep 2008 (20080921/ED)

ZCaplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

L1 STR

L5 397 SEA FILE=REGISTRY SSS FUL L1

L6 11 SEA FILE=ZCAPLUS ABB=ON L5

L6 ANSWER 1 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:6179 ZCAPLUS Full-text

DOCUMENT NUMBER: 148:121717

TITLE: Preparation of 1,4-diaryldihydropyrimidin-2-ones for treatment of pulmonary arterial hypertension.

INVENTOR(S): von Nussbaum, Franz; Gielen-Haertwig, Heike; Klein, Martina; Li, Volkhart; Meibom, Daniel; Sandner, Peter; Lustig, Klemens; Schaefer, Stefan

PATENT ASSIGNEE(S): Bayer Healthcare Aktiengesellschaft, Germany

SOURCE: Ger. Offen., 34pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

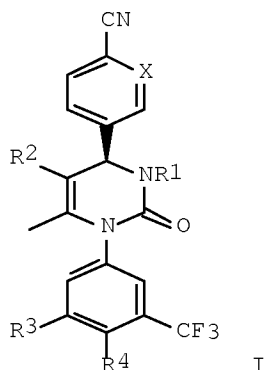
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----------------|------|----------|----------------------|----------|
| DE 102006031314 | A1 | 20080103 | DE 2006-102006031314 | 20060701 |
| WO 2008003412 | A1 | 20080110 | WO 2007-EP5579 | 20070625 |

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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: DE 2006-102006031314A 20060701
 OTHER SOURCE(S): MARPAT 148:121717
 GI



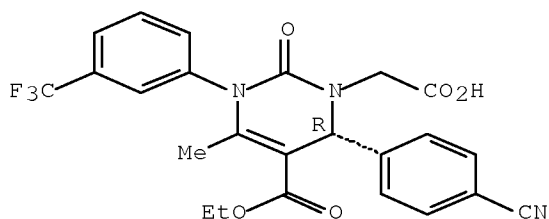
AB Use of title compds. [I; X = CH, N; R1 = (CH2)_nCO2R1 3-CH2C6H4CO2R1a, 4-CH2C6H4CO2R1a; n = 1, 2; R1a = H, alkyl; R2 = cyano, COR2a, CO2R2a; R2a = (substituted) alkyl, cycloalkyl; R3 = H, R4 = H, F, Cl; or R3 = F, Cl and R4 = H] for use in preparation of a drug for treatment of pulmonary arterial hypertension is claimed. Thus, 5-methylhexane-2,4-dione, 4-formylbenzonitrile, and 1-[3-(trifluoromethyl)phenyl]urea were heated with polyphosphoric acid in THF overnight at 80° to give a residue which was subjected to chiral chromatog. to give 8% 4-[(4R)-5-isobutyryl-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-1,2,3,4-tetrahydropyrimidin-4-yl]benzonitrile. I inhibited human neutrophil elastase with IC₅₀ = 0.9-20 nM.

IT 904958-43-6P 956487-28-8P 1000588-67-9P
 1000588-70-4P 1000588-73-7P 1000588-74-8P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of diaryldihydropyrimidinones for treatment of pulmonary arterial hypertension)

RN 904958-43-6 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

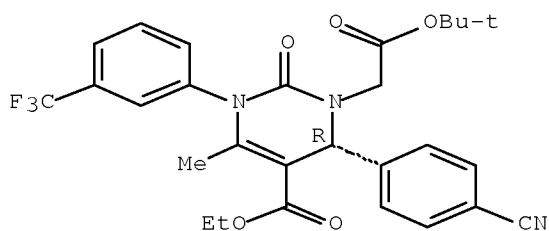
Absolute stereochemistry.



RN 956487-28-8 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, (6R)- (CA INDEX NAME)

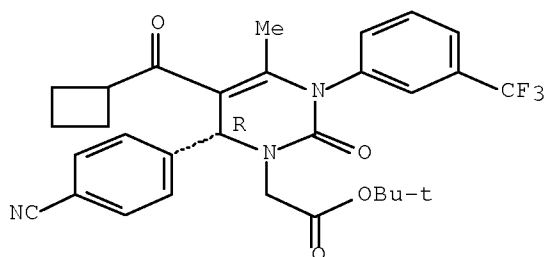
Absolute stereochemistry.



RN 1000588-67-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclobutylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, (6R)- (CA INDEX NAME)

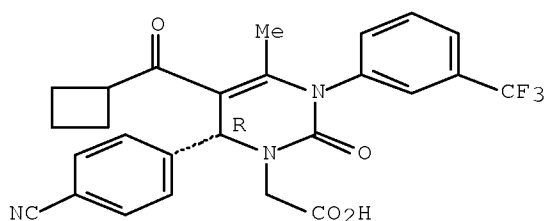
Absolute stereochemistry.



RN 1000588-70-4 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclobutylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

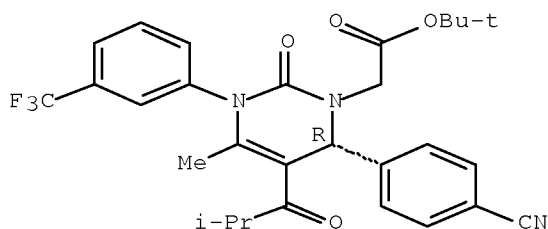
Absolute stereochemistry.



RN 1000588-73-7 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(2-methyl-1-oxopropyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, (6R)- (CA INDEX NAME)

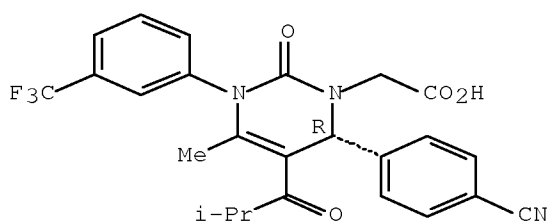
Absolute stereochemistry.



RN 1000588-74-8 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(2-methyl-1-oxopropyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.



IT 864150-67-4 864150-68-5 864250-45-3

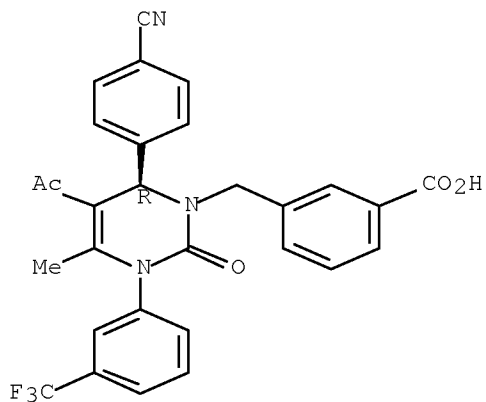
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of diaryldihydropyrimidinones for treatment of pulmonary arterial hypertension)

RN 864150-67-4 ZCAPLUS

CN Benzoic acid, 3-[[[(6R)-5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)

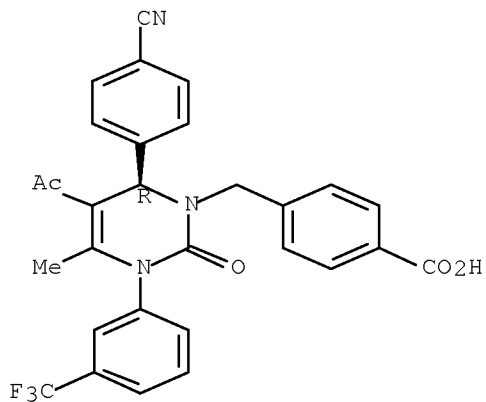
Absolute stereochemistry.



RN 864150-68-5 ZCAPLUS

CN Benzoic acid, 4-[[[(6R)-5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)

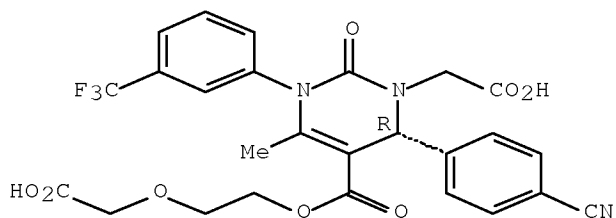
Absolute stereochemistry.



RN 864250-45-3 ZCAPLUS

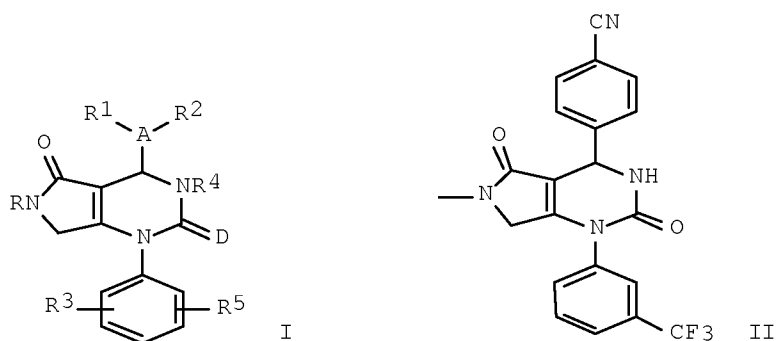
CN 1(2H)-Pyrimidineacetic acid, 5-[[2-(carboxymethoxy)ethoxy]carbonyl]-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 2 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2007:1300977 ZCAPLUS Full-text
 DOCUMENT NUMBER: 147:522270
 TITLE: Preparation of tetrahydropyrrolopyrimidinediones as
 human neutrophil elastase (HNE) inhibitors
 INVENTOR(S): Ray, Nicholas Charles; Finch, Harry; Edwards,
 Christine; O'Connor, Elizabeth
 PATENT ASSIGNEE(S): Argenta Discovery Limited, UK
 SOURCE: PCT Int. Appl., 73pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|----------|-------------------|------------|
| WO 2007129060 | A1 | 20071115 | WO 2007-GB1638 | 20070503 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| PRIORITY APPLN. INFO.: | | | GB 2006-8844 | A 20060504 |
| | | | GB 2006-12544 | A 20060623 |
| OTHER SOURCE(S): | | | MARPAT 147:522270 | |
| GI | | | | |



AB Title compds. [I; A = aryl, heteroaryl; D = O, S; R1-R3 = H, OH, halo, NO2, cyano, alkenyl, alkynyl, alkenyloxy, (substituted) alkyl, alkoxy; R, R4 = Xm(A1)pQn(A2)q(X1)kZ; A1, A2 = (substituted) alkylene, alkenylene optionally containing O, S, NRa; Q = O, S, SO, SO2, NRa, NRaSO2, CO2, etc.; X = CO, SO2, CO2, CONRa, SO2NRa; Ra = H, alkyl, cycloalkyl; X1 = O, S, NH; Z = H,

(substituted) carbocyclyl, heterocyclyl; k, m, n, p, q = 0, 1], were prepared
Thus, title compound (II) was prepared in 3 steps from 3,5-difluorophenylurea,
4-cyanobenzaldehyde, Et acetoacetate, and methylamine. Most I inhibited HNE
in the range of 1-50 nM.

IT 956487-15-3P 956487-16-4P 956487-17-5P
956487-18-6P 956487-19-7P 956487-20-0P
956487-21-1P 956487-22-2P 956487-23-3P
956487-28-8P 956487-29-9P 956487-38-0P
956487-39-1P 956487-40-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

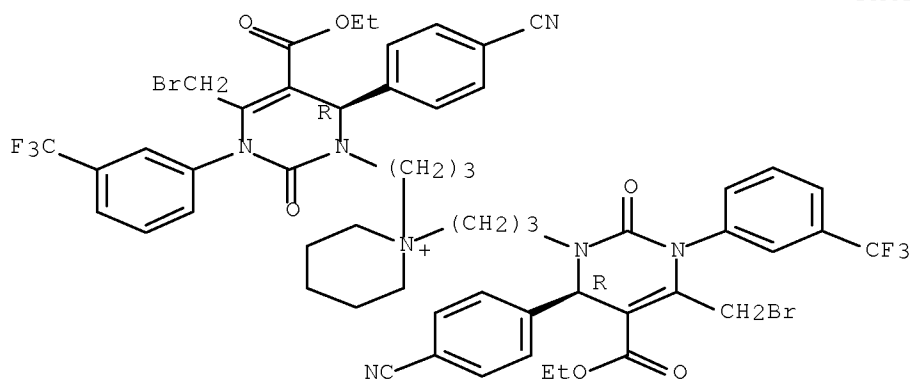
(preparation of tetrahydropyrrolopyrimidinediones as human neutrophil
elastase inhibitors)

RN 956487-15-3 ZCAPLUS

CN Piperidinium, 1,1-bis[3-[(6R)-4-(bromomethyl)-6-(4-cyanophenyl)-5-
(ethoxycarbonyl)-3,6-dihydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-
pyrimidinyl]propyl]-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

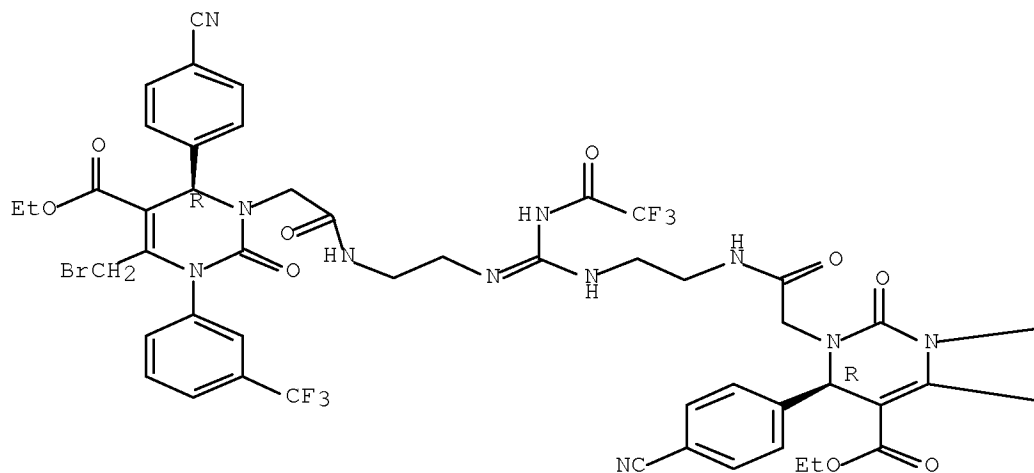


RN 956487-16-4 ZCAPLUS

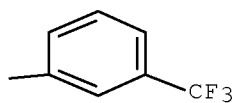
CN 5-Pyrimidinecarboxylic acid, 1,1'-[2,12-dioxo-7-[(2,2,2-
trifluoroacetyl)amino]-3,6,8,11-tetraazatridec-6-ene-1,13-diyl]bis[4-
(bromomethyl)-6-(4-cyanophenyl)-1,2,3,6-tetrahydro-2-oxo-3-[3-
(trifluoromethyl)phenyl]-, 5,5'-diethyl ester, (6R,6'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



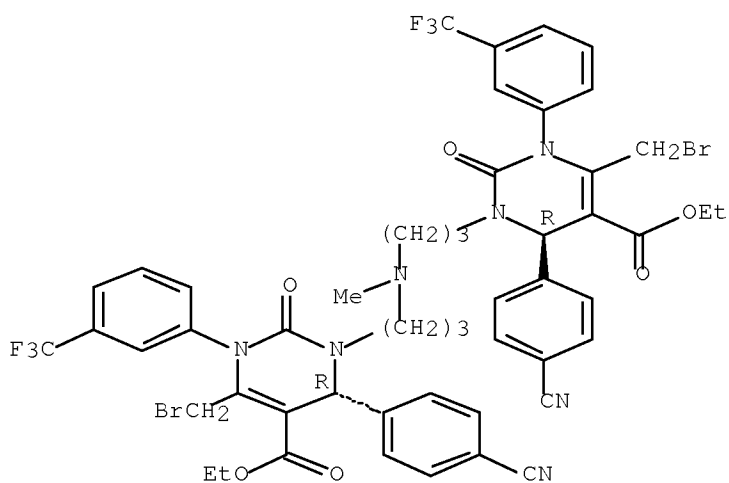
PAGE 1-B

-CH₂Br

RN 956487-17-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[(methylimino)di-3,1-propanediyl]bis[4-(bromomethyl)-6-(4-cyanophenyl)-1,2,3,6-tetrahydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 5,5'-diethyl ester, (6R,6'R)- (CA INDEX NAME)

Absolute stereochemistry.

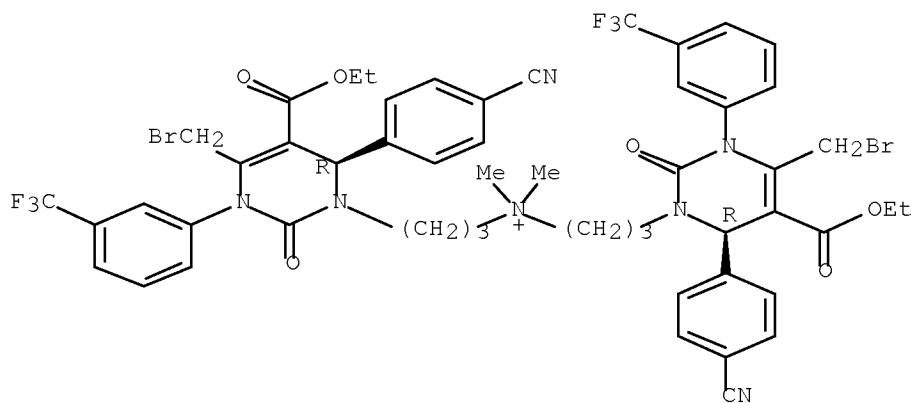


RN 956487-18-6 ZCAPLUS

CN 1(2H)-Pyrimidinepropanaminium, 4-(bromomethyl)-N-[3-[(6R)-4-(bromomethyl)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-N,N-dimethyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, iodide (1:1), (6R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

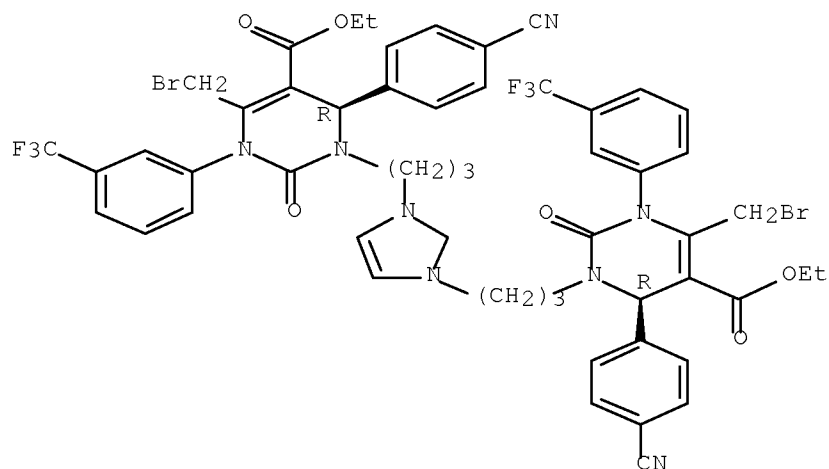


RN 956487-19-7 ZCAPLUS

CN 1H-Imidazolium, 1,3-bis[3-[(6R)-4-(bromomethyl)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



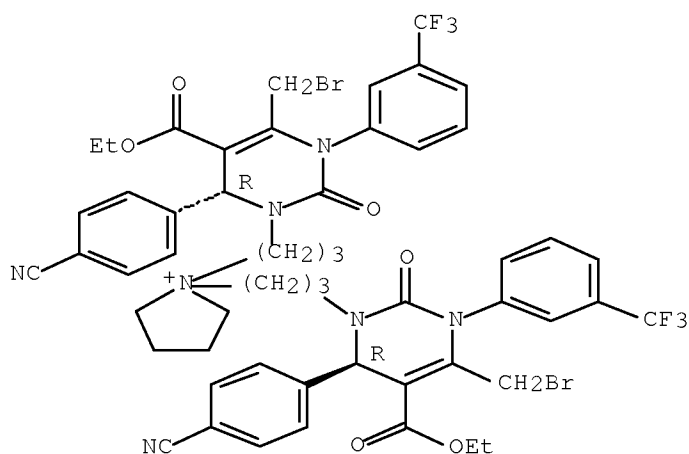
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 956487-20-0 ZCAPLUS

CN Pyrrolidinium, 1,1-bis[3-[(6R)-4-(bromomethyl)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

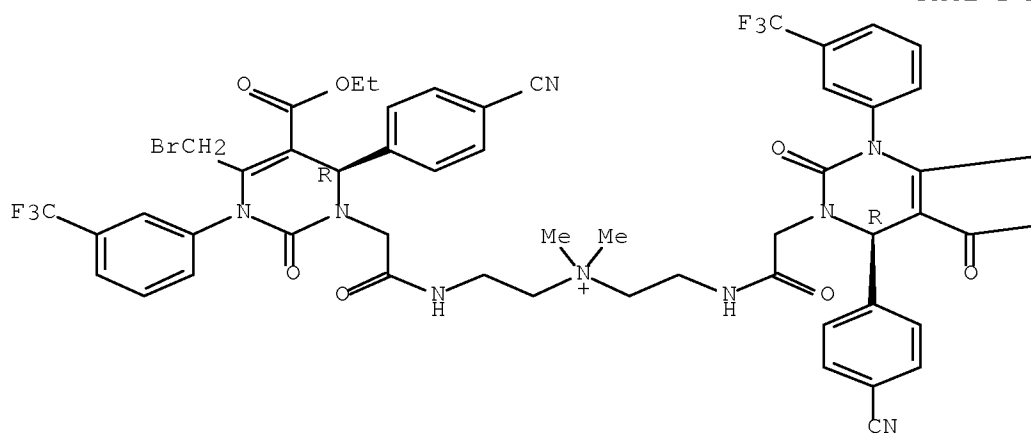




RN 956487-21-1 ZCAPLUS

CN Ethanaminium, 2-[[2-[(6R)-4-(bromomethyl)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[(6R)-4-(bromomethyl)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.



—CH₂Br

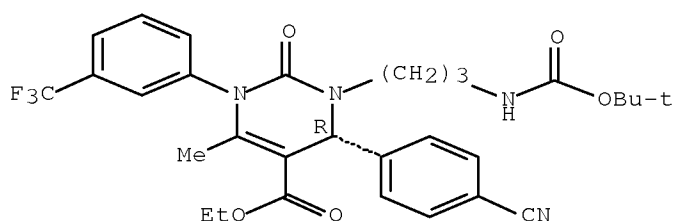
—OEt



RN 956487-22-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[3-[[[(1,1-dimethylethoxy)carbonyl]amino]propyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

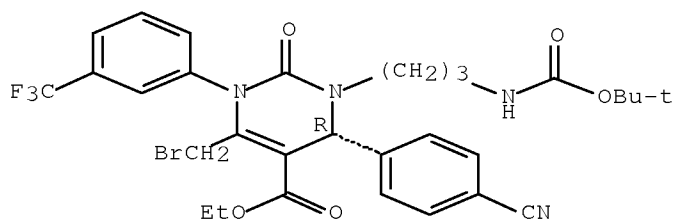
Absolute stereochemistry.



RN 956487-23-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(bromomethyl)-4-(4-cyanophenyl)-3-[3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]-1,2,3,4-tetrahydro-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

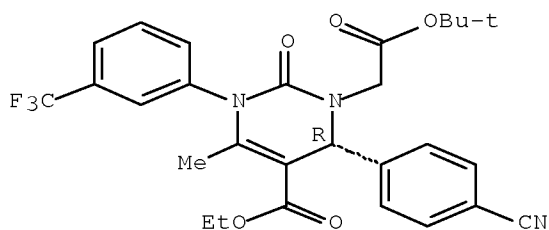
Absolute stereochemistry.



RN 956487-28-8 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, (6R)- (CA INDEX NAME)

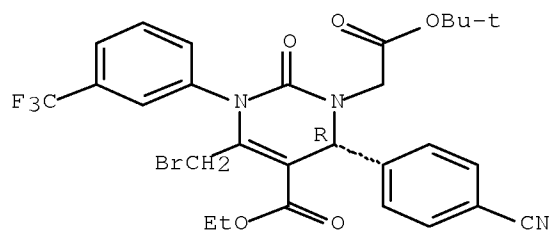
Absolute stereochemistry.



RN 956487-29-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 4-(bromomethyl)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, (6R)- (CA INDEX NAME)

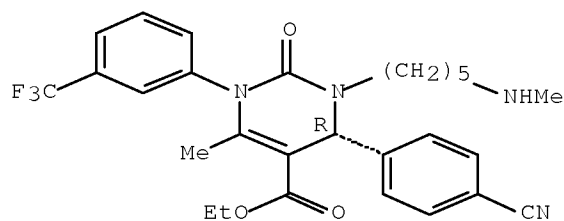
Absolute stereochemistry.



RN 956487-38-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[5-(methylamino)pentyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

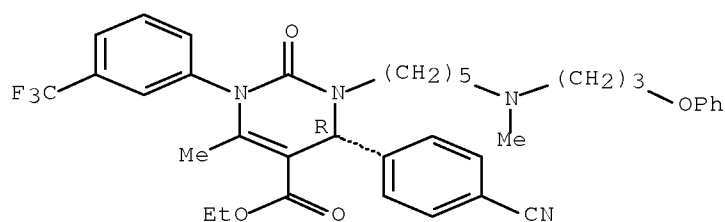
Absolute stereochemistry.



RN 956487-39-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[5-[methyl(3-phenoxypropyl)amino]pentyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

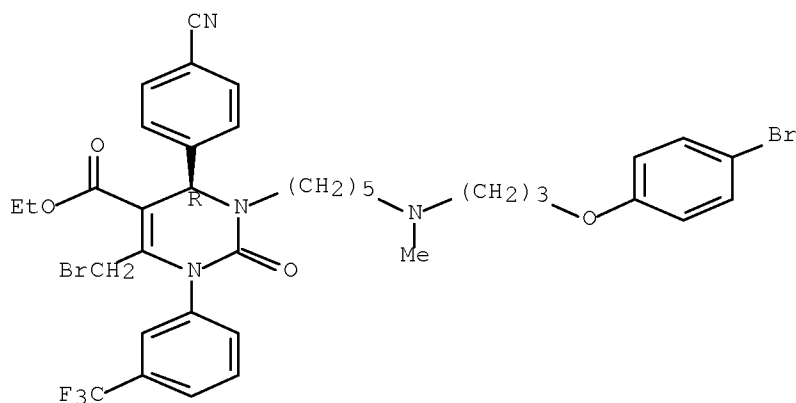
Absolute stereochemistry.



RN 956487-40-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(bromomethyl)-3-[5-[3-(4-bromophenoxy)propyl]methylamino]pentyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2006:1356757 ZCAPLUS Full-text
 DOCUMENT NUMBER: 146:100714
 TITLE: Preparation of dihydropyrimidone multimers as human neutrophil elastase inhibitors
 INVENTOR(S): Finch, Harry; Edwards, Christine; Ray, Nicholas Charles; Fitzgerald, Mary Frances
 PATENT ASSIGNEE(S): Argenta Discovery Ltd., UK
 SOURCE: PCT Int. Appl., 59pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|----------|------------------|------------|
| WO 2006136857 | A1 | 20061228 | WO 2006-GB2337 | 20060626 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| EP 1893584 | A1 | 20080305 | EP 2006-755623 | 20060626 |
| R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR | | | | |
| IN 2007DN10018 | A | 20080711 | IN 2007-DN10018 | 20071224 |
| CN 101243055 | A | 20080813 | CN 2006-80030331 | 20080220 |
| PRIORITY APPLN. INFO.: | | | GB 2005-12940 | A 20050624 |
| | | | WO 2006-GB2337 | W 20060626 |

OTHER SOURCE(S): MARPAT 146:100714
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. represented by the formula M-L-M, wherein L is a linker and each M is independently a group of formula I [A = (hetero)aryl; D = O or S; R1-R3 = independently H, halo, nitro, etc.; R4 = OH, alkyl(carbonyl), amino, etc.; Y1-Y5 = independently C or N, with the proviso that the ring in which they are comprised contains no more than 2 N atoms; R5 = (un)substituted alkyl, -O-alkyl-O-alkyl or amino; R6 = halo, nitro, cyano, etc.; and pharmaceutically acceptable salts, solvates or N-oxides thereof], were prepared as human neutrophil elastase (HNE) inhibitors. For example, II was provided in a multi-step synthesis starting from the reaction of 3-(trifluoromethyl)phenylurea with 4-cyanobenzaldehyde. I were tested for inhibitory activity towards HNE with IC50 values of 1-1000 nM. Thus, I and their pharmaceutical compns. are useful as human neutrophil elastase inhibitors for the treatment of respiratory diseases (no data).

IT 917813-97-9P 917813-99-1P 917814-01-8P
917814-02-9P

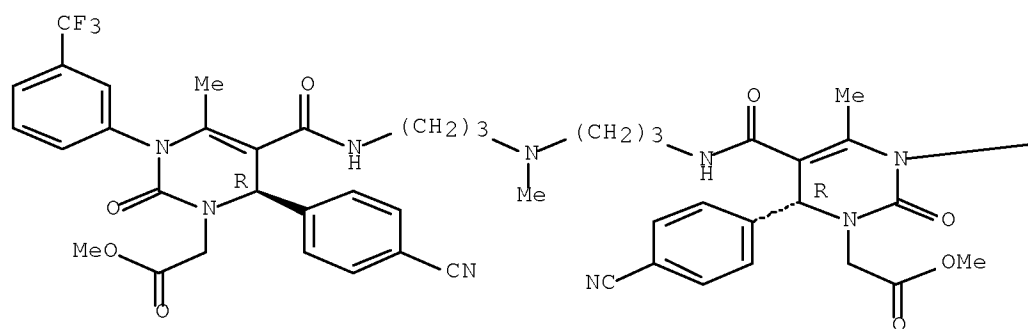
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of dihydropyrimidone multimers as human neutrophil elastase inhibitors)

RN 917813-97-9 ZCAPLUS

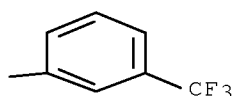
CN 1(2H)-Pyrimidineacetic acid, 5,5'-[(methylimino)bis(3,1-propanediyliminocarbonyl)]bis[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1'-dimethyl ester, (6R,6'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

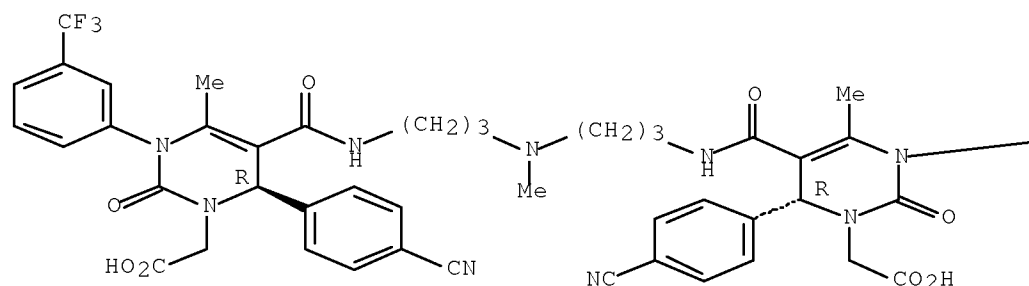


RN 917813-99-1 ZCAPLUS

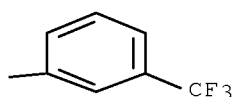
CN 1(2H)-Pyrimidineacetic acid, 5,5'-[(methylimino)bis(3,1-propanediyliminocarbonyl)]bis[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R,6'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

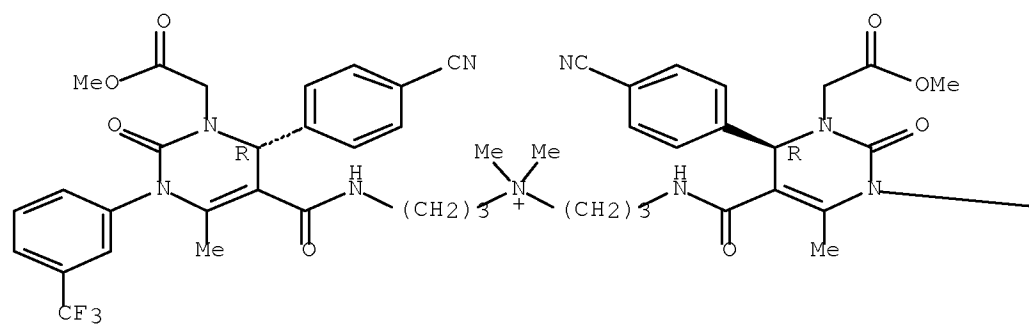


RN 917814-01-8 ZCAPLUS

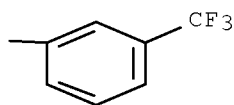
CN 1-Propanaminium, 3-[[[(4R)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-(2-methoxy-2-oxoethyl)-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]amino]-N-[3-[[[(4R)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-(2-methoxy-2-oxoethyl)-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]amino]propyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



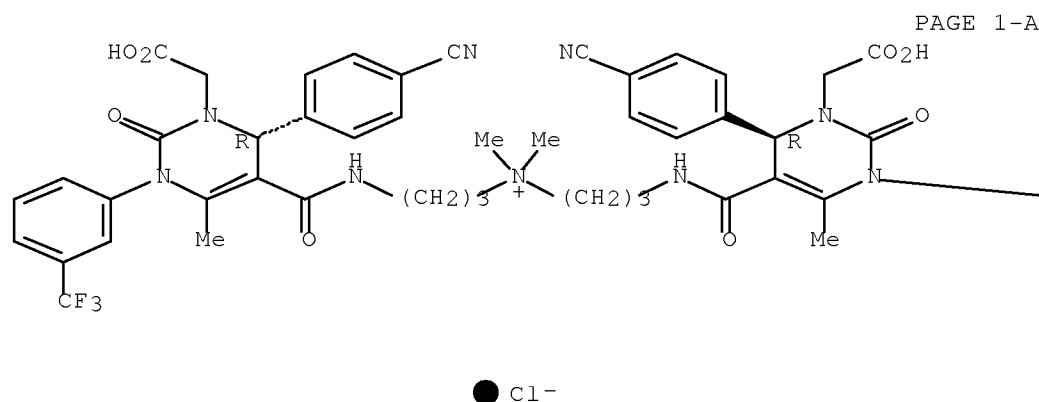
PAGE 1-B



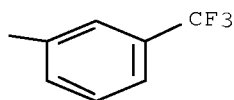
RN 917814-02-9 ZCAPLUS

CN 1-Propanaminium, 3-[[[(4R)-3-(carboxymethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]amino]-N-[3-[[[(4R)-3-(carboxymethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]amino]propyl]-N,N-dimethyl-, chloride (1:1) (CA INDEX NAME)

Absolute stereochemistry.



PAGE 1-B



IT 917814-00-7P 917814-03-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

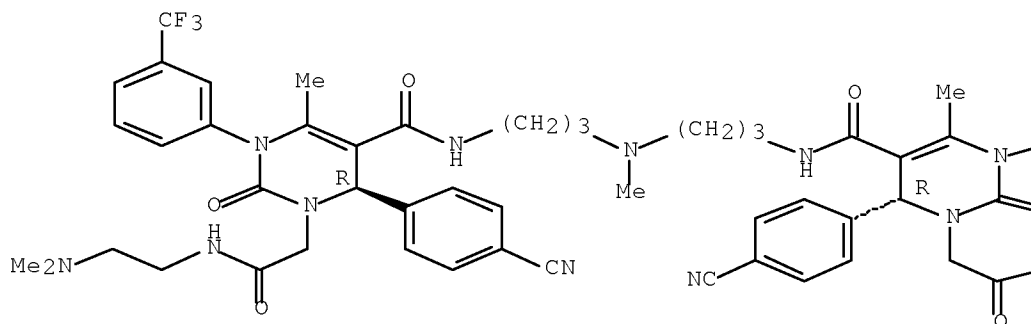
(preparation of dihydropyrimidone multimers as human neutrophil elastase
inhibitors)

RN 917814-00-7 ZCAPLUS

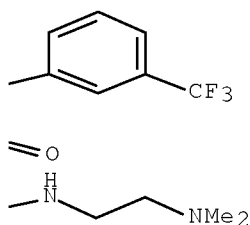
CN 1(2H)-Pyrimidineacetamide, 5,5'-[(methylimino)bis(3,1-
propanediyliminocarbonyl)]bis[6-(4-cyanophenyl)-N-[2-(dimethylamino)ethyl]-
3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R,6'R)- (CA
INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

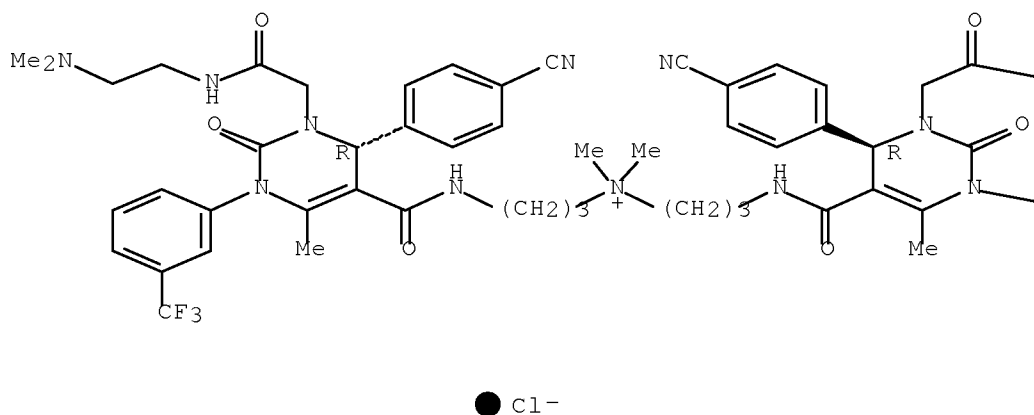


RN 917814-03-0 ZCAPLUS

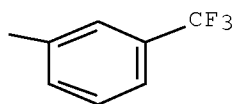
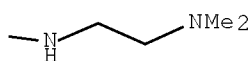
CN 1-Propanaminium, 3-[[[(4R)-4-(4-cyanophenyl)-3-[2-[[2-(
(dimethylamino)ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-
1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]amino]-N-[3-[[[(4R)-4-
(4-cyanophenyl)-3-[2-[[2-(dimethylamino)ethyl]amino]-2-oxoethyl]-1,2,3,4-
tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-
pyrimidinyl]carbonyl]amino]propyl]-N,N-dimethyl-, chloride (1:1) (CA
INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

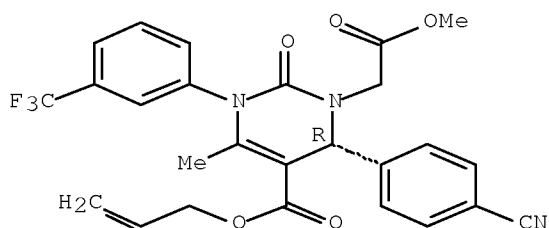


PAGE 1-B



IT 917814-23-4P 917814-24-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of dihydropyrimidone multimers as human neutrophil elastase
 inhibitors)
 RN 917814-23-4 ZCAPLUS
 CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-
 5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-, methyl
 ester, (6R)- (CA INDEX NAME)

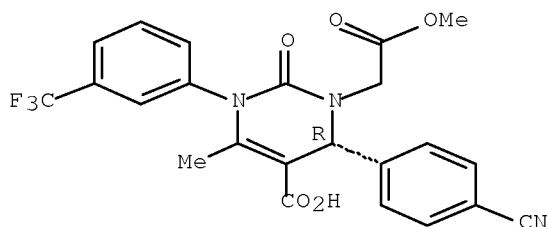
Absolute stereochemistry.



RN 917814-24-5 ZCAPLUS
 CN 1(2H)-Pyrimidineacetic acid, 5-carboxy-6-(4-cyanophenyl)-3,6-dihydro-4-

methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1-methyl ester, (6R)- (CA
INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:796025 ZCAPLUS Full-text

DOCUMENT NUMBER: 145:211067

TITLE: Multimers of tetrahydropyrimidinone compounds as
elastase inhibitors and their preparation,
pharmaceutical compositions, and use for treatment of
respiratory diseases

INVENTOR(S): Finch, Harry; Edwards, Christine; Ray, Nicholas
Charles; O'Connor, Elizabeth Anne; Fitzgerald, Mary F.

PATENT ASSIGNEE(S): Argenta Discovery Ltd, UK

SOURCE: PCT Int. Appl., 132 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|-----------------|----------|
| WO 2006082412 | A2 | 20060810 | WO 2006-GB361 | 20060203 |
| WO 2006082412 | A3 | 20061012 | | |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | |
| RW: | AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| AU 2006210730 | A1 | 20060810 | AU 2006-210730 | 20060203 |
| CA 2595801 | A1 | 20060810 | CA 2006-2595801 | 20060203 |
| EP 1856059 | A2 | 20071121 | EP 2006-709612 | 20060203 |
| R: | AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR | | | |
| JP 2008528670 | T | 20080731 | JP 2007-553695 | 20060203 |
| IN 2007DN05905 | A | 20070817 | IN 2007-DN5905 | 20070727 |

CN 101151252 A 20080326 CN 2006-80009856 20070926
 PRIORITY APPLN. INFO.: GB 2005-2258 A 20050203
 WO 2006-GB361 W 20060203
 OTHER SOURCE(S): MARPAT 145:211067
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

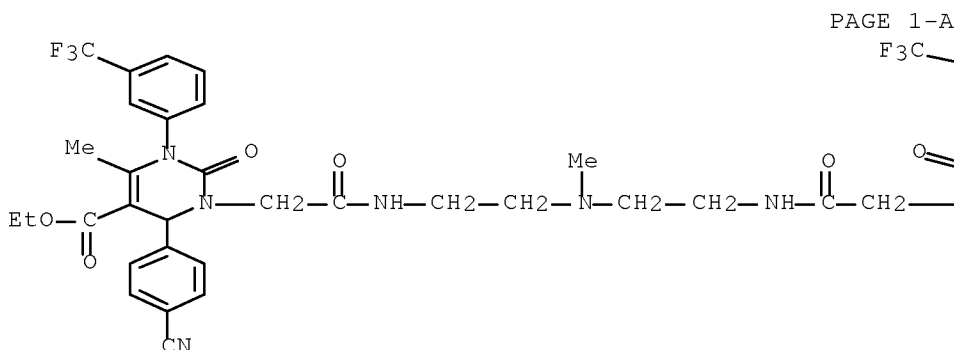
AB A compound of formula I is useful in therapy, e.g. of respiratory diseases. Compds. of formula I wherein L is a linker; each A are independently (un)substituted (hetero)aryl; D is O or S; each Y1 - Y5 are independently CH, CR3, CR6 or N, with the proviso that one of them is CR3, one CR6 and not more than two N per ring; each R3 are independently H, halo, NO2, CN, (un)substituted C1-6 alkyl, OH, or (un)substituted C1-6 alkoxy; each R4 are independently COCF3, (un)substituted C1-6 alkylcarbonyl, (un)substituted C1-6 alkoxy carbonyl, (un)substituted C1-6 alkenyloxycarbonyl, hydroxycarbonyl, CONH2 and derivs., (un)substituted (hetero)aroyl, etc.; each R5 are independently (un)substituted C1-4 alkyl or amino; each R6 are independently halo, NO2, CN, (un)substituted C1-6 alkyl, OH, or (un)substituted C1-6 alkoxy; and their pharmaceutically acceptable salts, solvates or N-oxides thereof are claimed. Example compound II was prepared by N-alkylation of compound III with 1,12-dibromododecane. The invention compds. were evaluated for their elastase inhibitory activity. The tested compds. were shown to have desirable HNE inhibitory activity (no data).

IT 904957-71-7P 904957-72-8P 904957-86-4P
 904958-07-2P 904958-35-6P

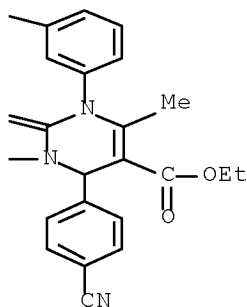
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (drug candidate and intermediate; preparation of multimers of tetrahydropyrimidinone compds. as elastase inhibitors useful in the treatment of respiratory diseases)

RN 904957-71-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-[[2-[[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



PAGE 1-B

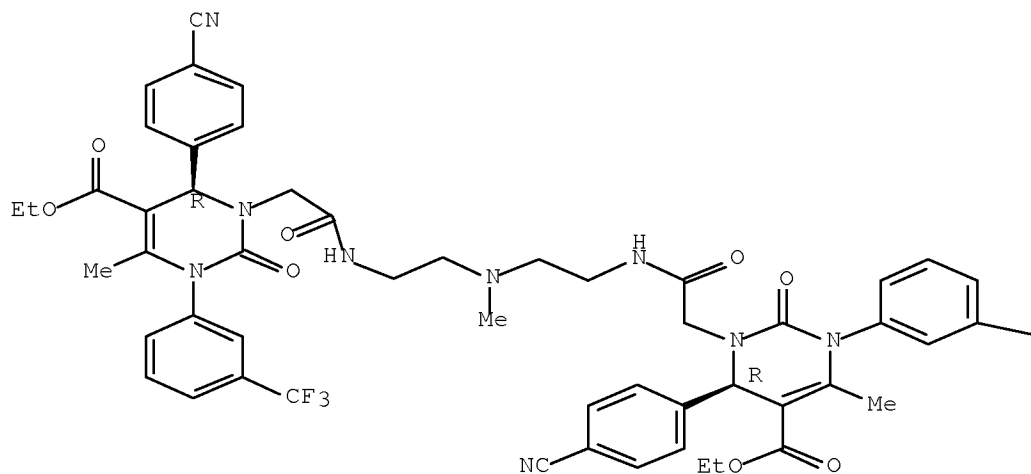


RN 904957-72-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-[[2-[[2-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

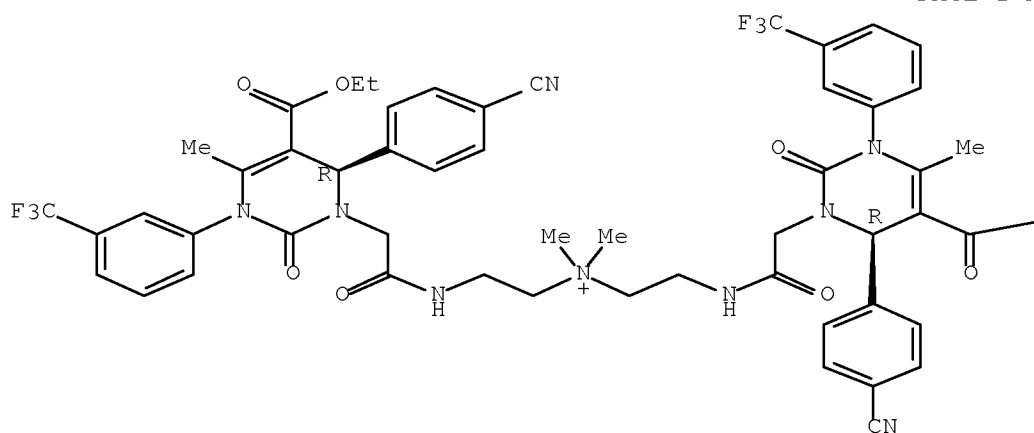


—CF₃

RN 904957-86-4 ZCAPLUS

CN Ethanaminium, 2-[[2-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.



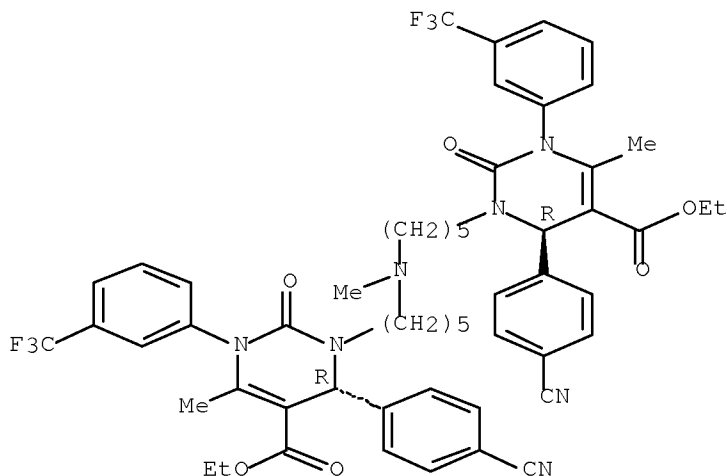
—OEt

● I⁻

RN 904958-07-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[(methylimino)di-5,1-pentanediy]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

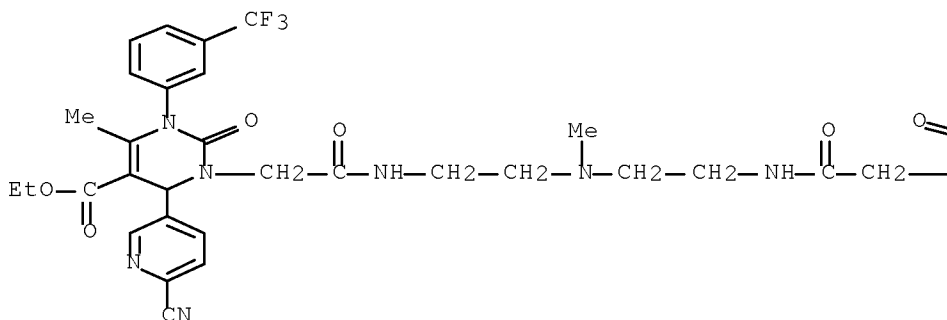
Absolute stereochemistry.



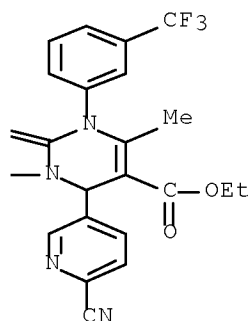
RN 904958-35-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(6-cyano-3-pyridinyl)-3-[2-[[2-[[2-[[2-[6-(6-cyano-3-pyridinyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



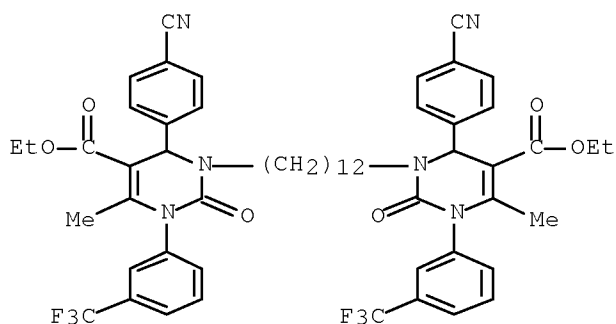
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 904958-39-0P 904958-41-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(drug candidate; preparation of multimers of tetrahydropyrimidinone compds.
 as elastase inhibitors useful in the treatment of respiratory diseases)

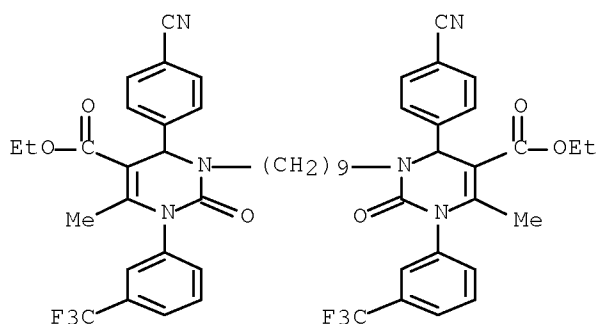
RN 904957-62-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,12-dodecanediyl)bis[6-(4-cyanophenyl)-
 1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl
 ester (9CI) (CA INDEX NAME)



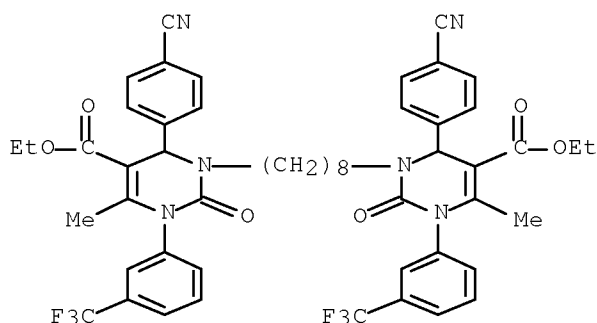
RN 904957-63-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,9-nonanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



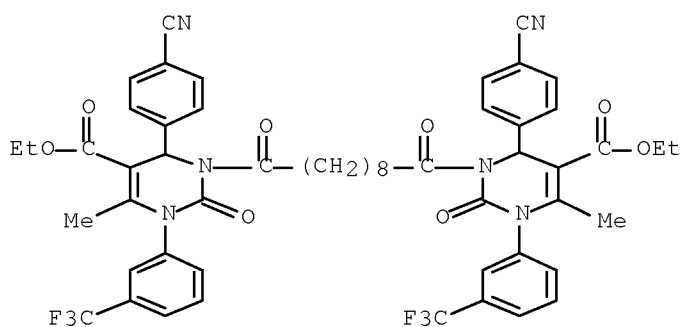
RN 904957-64-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,8-octanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



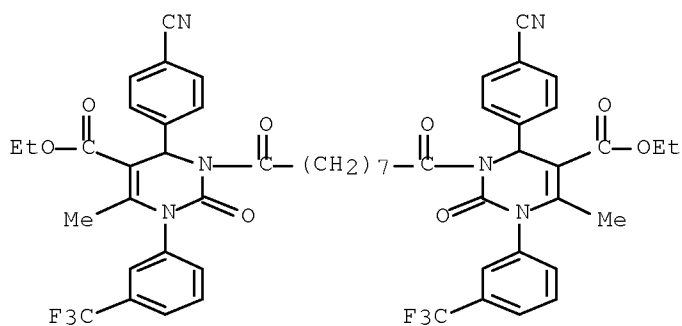
RN 904957-65-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,10-dioxo-1,10-decanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



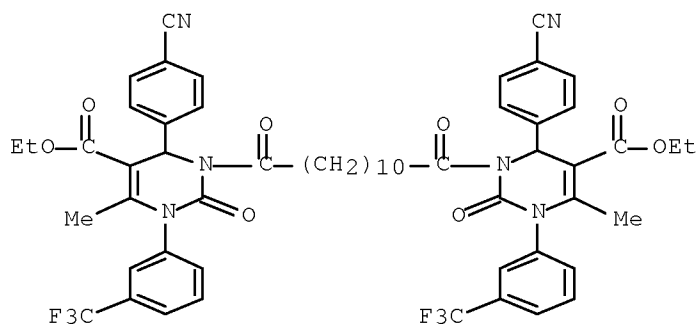
RN 904957-66-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,9-dioxo-1,9-nonanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 904957-67-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,12-dioxo-1,12-dodecanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

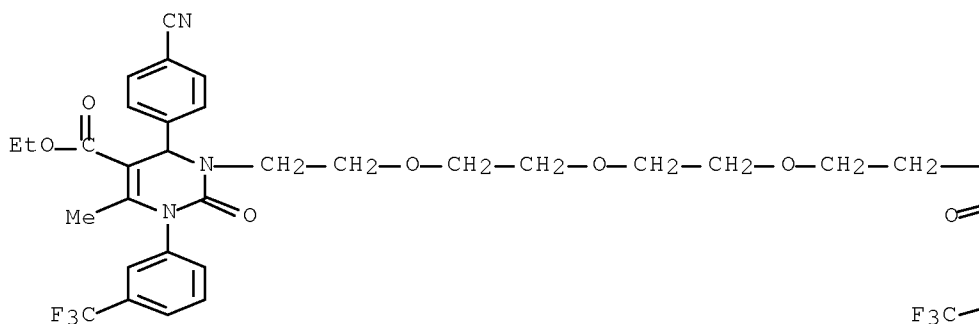


RN 904957-68-2 ZCAPLUS

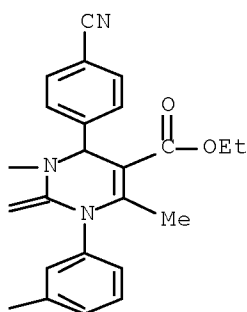
CN 5-Pyrimidinecarboxylic acid, 1,1'-[oxybis(2,1-ethanedioxy-2,1-

ethanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

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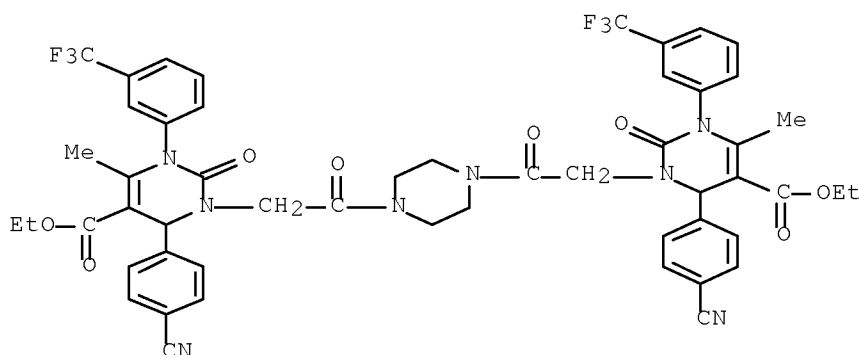


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RN 904957-69-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

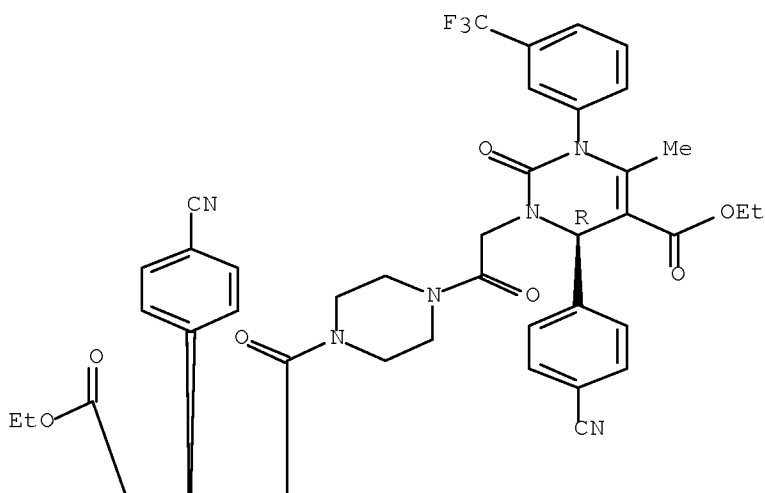


RN 904957-70-6 ZCAPLUS

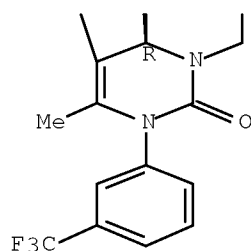
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[2-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

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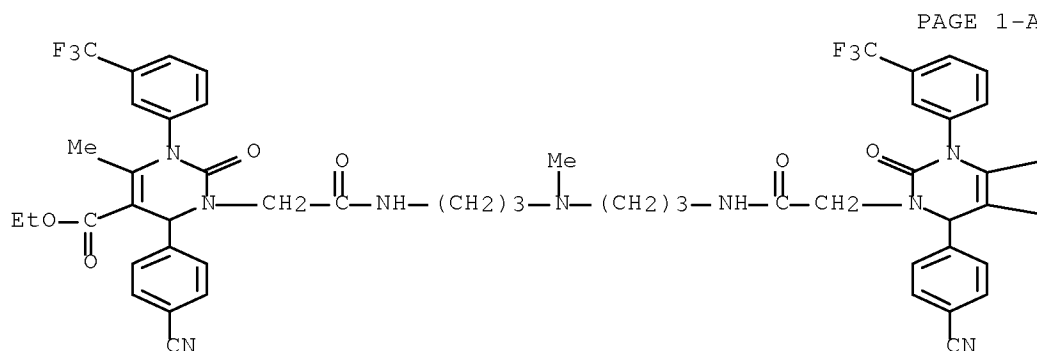


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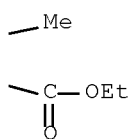


RN 904957-73-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[3-[3-[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]propyl]methylamino]propyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

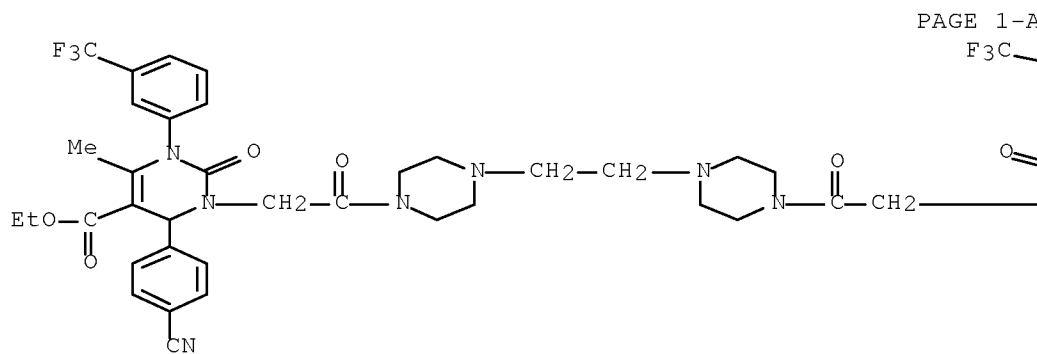


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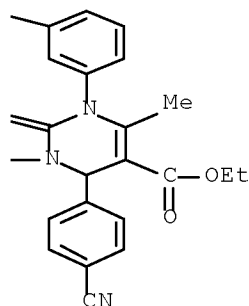


RN 904957-74-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[2-[4-[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]ethyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



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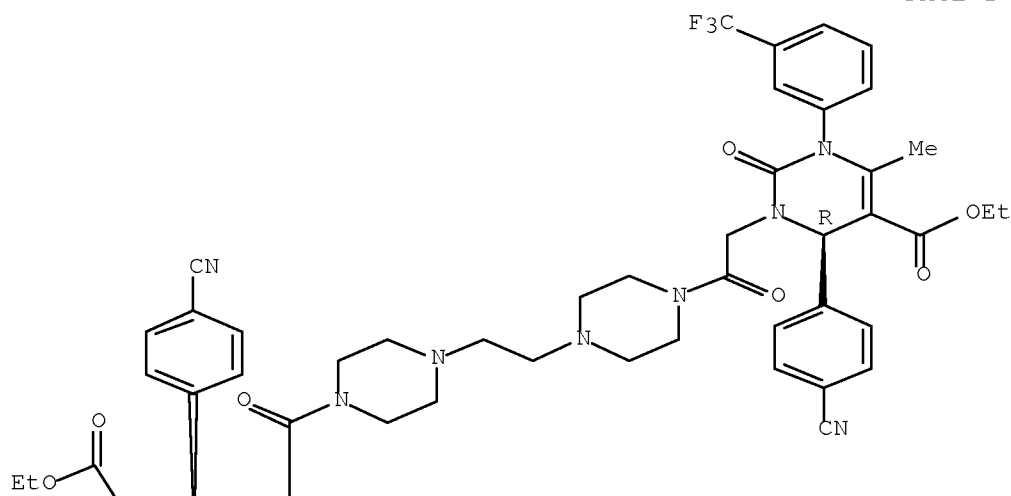


RN 904957-75-1 ZCAPLUS

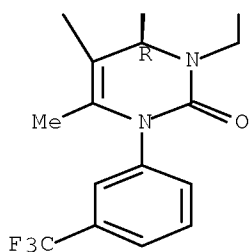
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[2-[4-[2-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]ethyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

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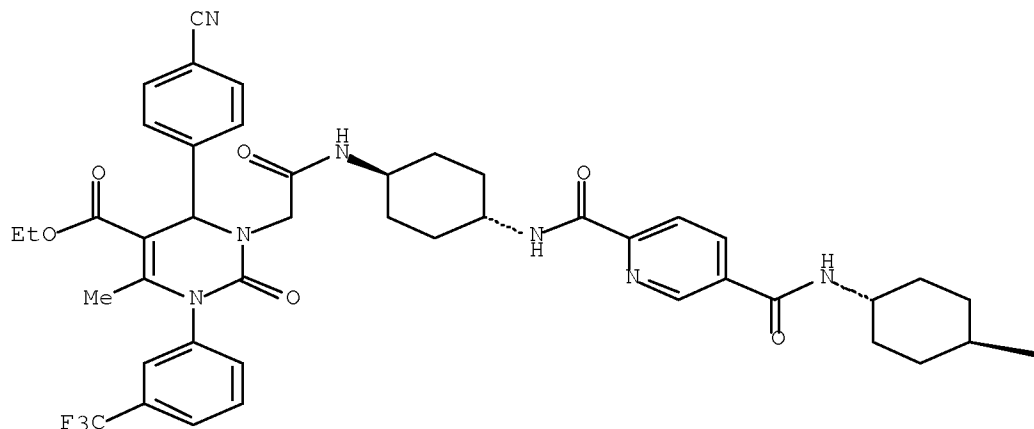


RN 904957-76-2 ZCAPLUS

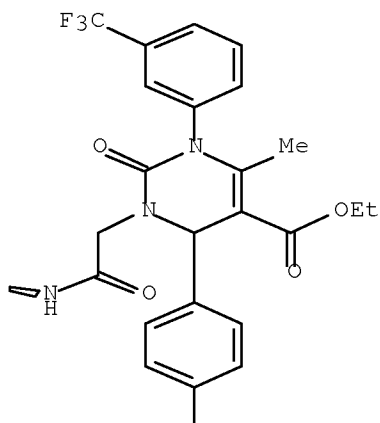
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[trans-4-[[[5-[[[trans-4-[[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]cyclohexyl]amino]carbonyl]-2-pyridinyl]carbonyl]amino]cyclohexyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

Relative stereochemistry.

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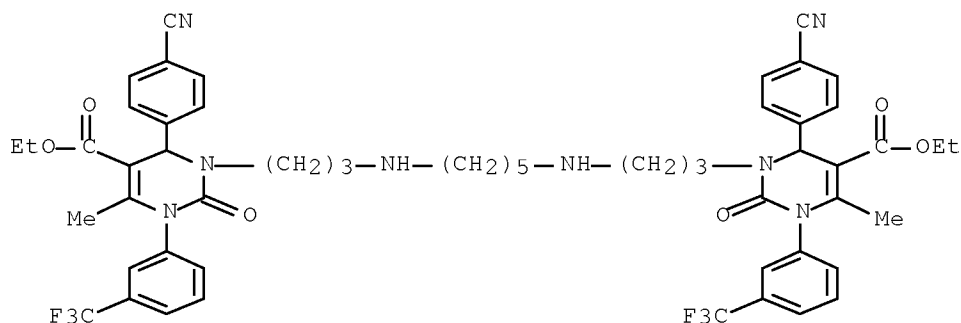


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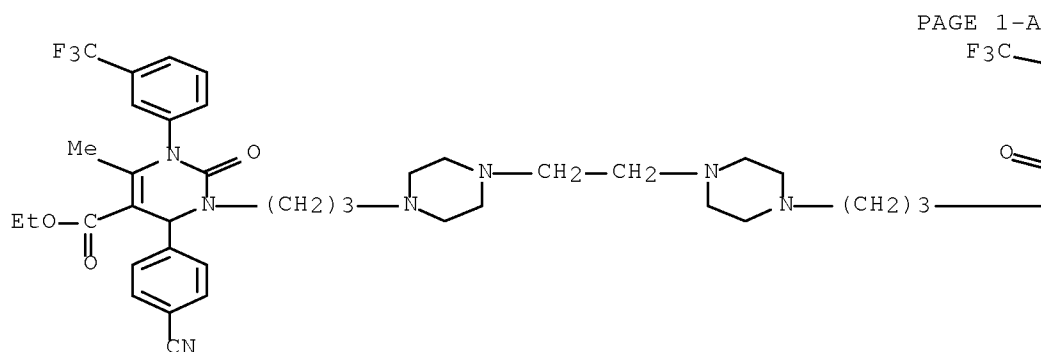
RN 904957-77-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,5-pentanediy]bis(imino-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)



RN 904957-78-4 ZCAPLUS

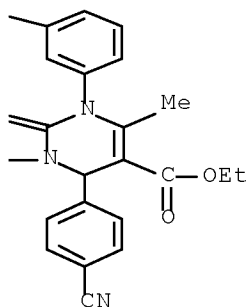
CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,2-ethanediyl]bis(4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



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F3C

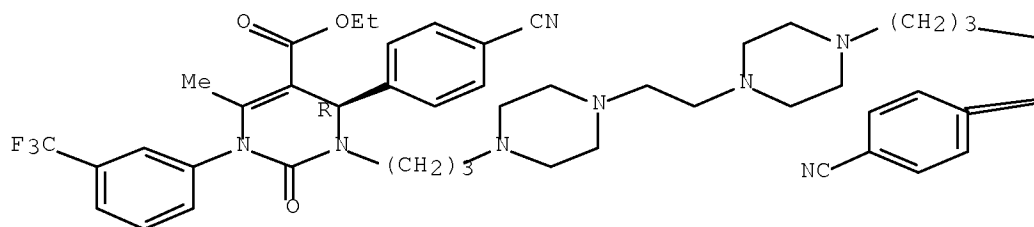
PAGE 1-B



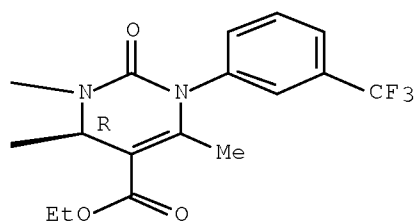
RN 904957-79-5 ZCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,2-ethanediylbis(4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

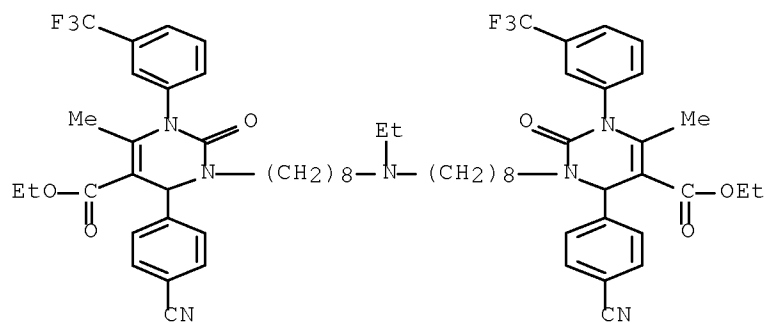
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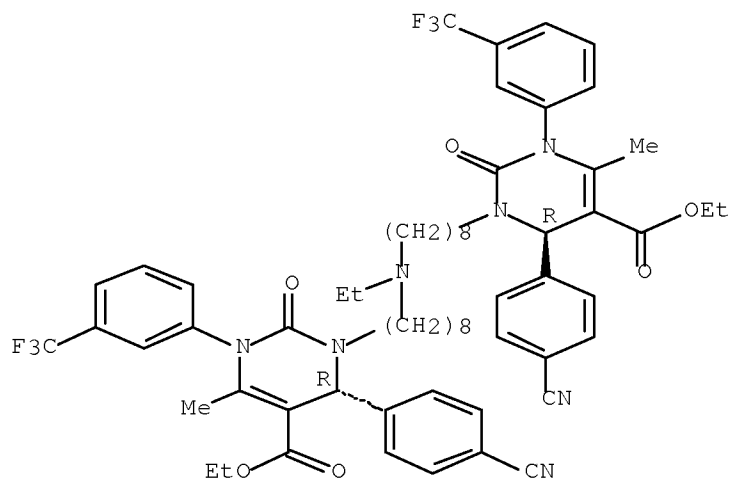
RN 904957-80-8 ZCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 1,1'-[(ethylimino)di-8,1-octanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 904957-81-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[(ethylimino)di-8,1-octanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



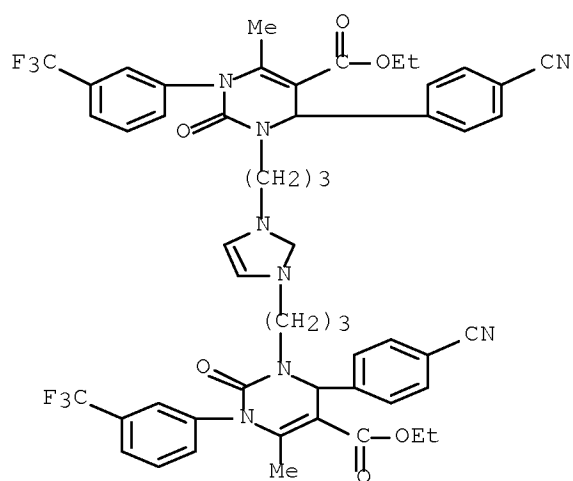
RN 904957-83-1 ZCAPLUS

CN 1H-Imidazolium, 1,3-bis[3-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 904957-82-0

CMF C53 H49 F6 N8 O6

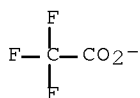


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

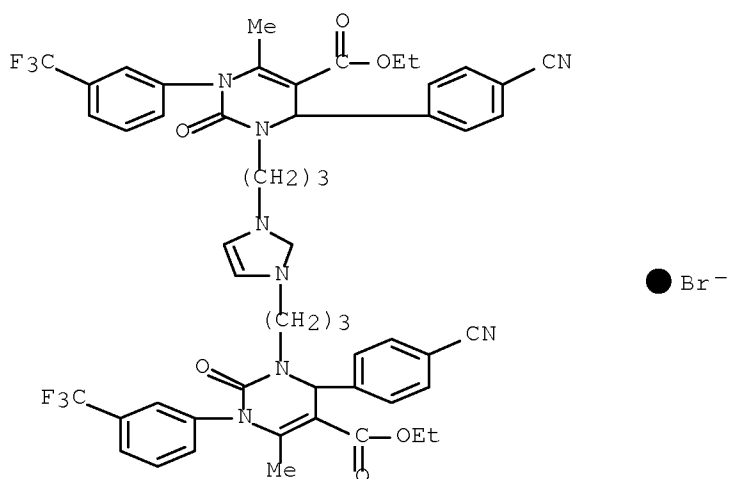
CRN 14477-72-6

CMF C2 F3 O2



RN 904957-84-2 ZCAPLUS

CN 1H-Imidazolium, 1,3-bis[3-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, bromide (1:1) (CA INDEX NAME)

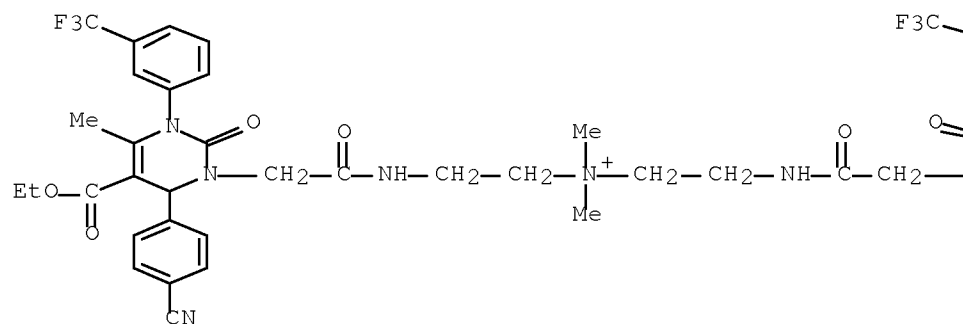


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

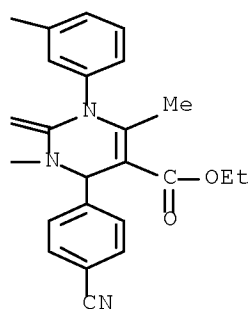
RN 904957-85-3 ZCAPLUS

CN Ethanaminium, 2-[[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

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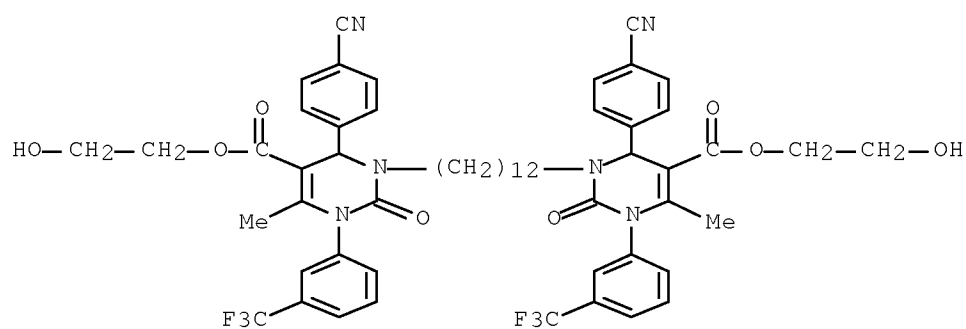


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RN 904957-87-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,12-dodecanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis(2-hydroxyethyl) ester (9CI) (CA INDEX NAME)

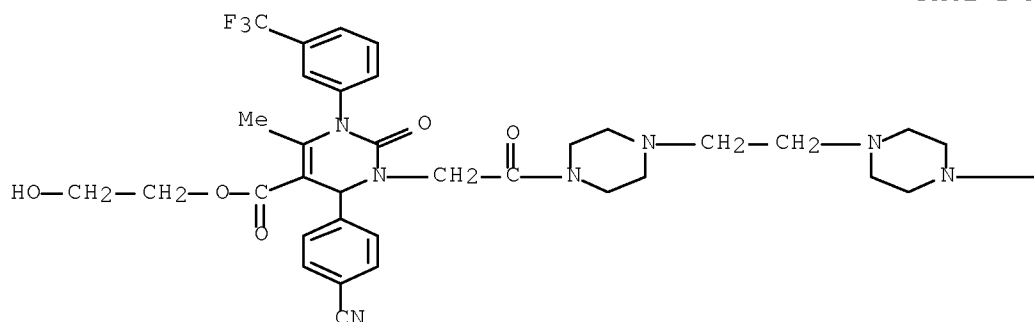


RN 904957-88-6 ZCAPLUS

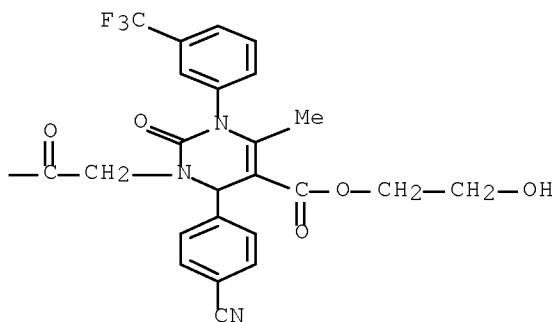
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[2-[4-[2-[6-(4-cyanophenyl)-3,6-dihydro-5-[(2-hydroxyethoxy)carbonyl]-4-methyl-2-oxo-3-[3-

(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]ethyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-hydroxyethyl ester (CA INDEX NAME)

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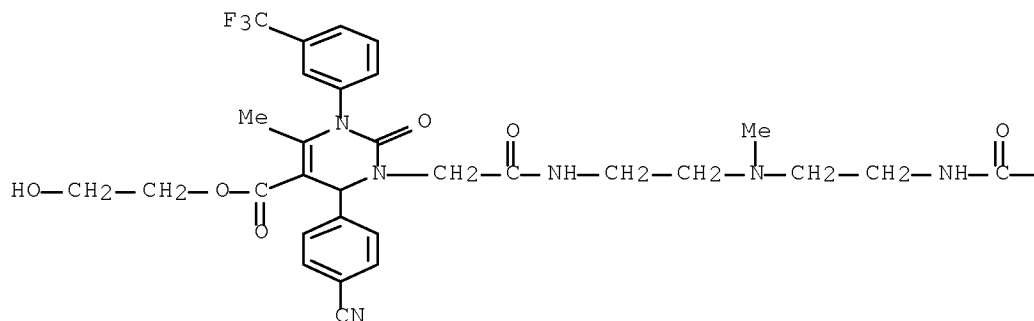
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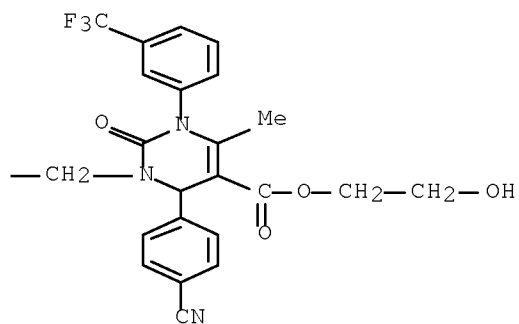
RN 904957-89-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-[[2-[[2-[6-(4-cyanophenyl)-3,6-dihydro-5-[(2-hydroxyethoxy)carbonyl]-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-hydroxyethyl ester (CA INDEX NAME)

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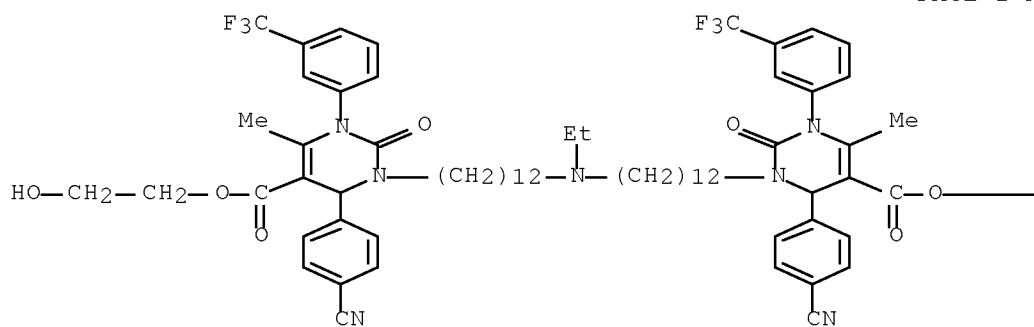
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RN 904957-90-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[(ethylimino)di-12,1-dodecanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis(2-hydroxyethyl) ester (9CI) (CA INDEX NAME)

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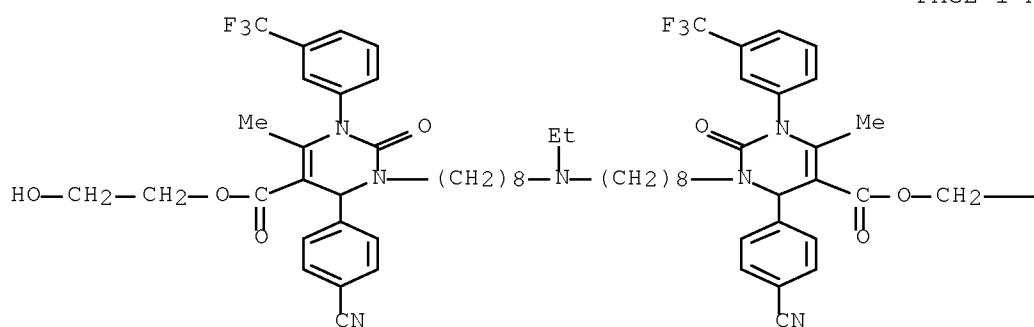


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—CH₂—CH₂—OH

RN 904957-91-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[(ethylimino)di-8,1-octanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis(2-hydroxyethyl) ester (9CI) (CA INDEX NAME)



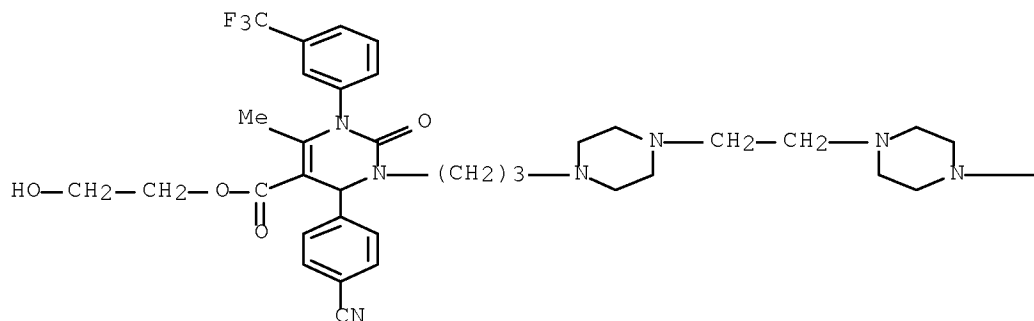
PAGE 1-B

—CH₂—OH

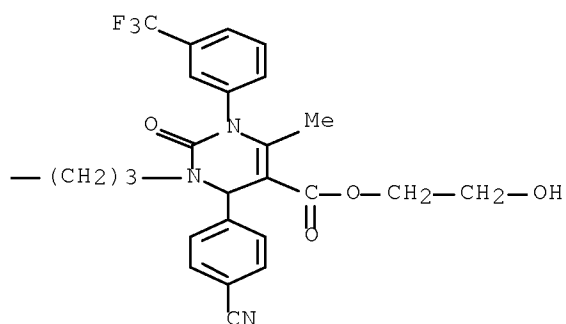
RN 904957-92-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,2-ethanediylbis(4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis(2-hydroxyethyl) ester (9CI) (CA INDEX NAME)

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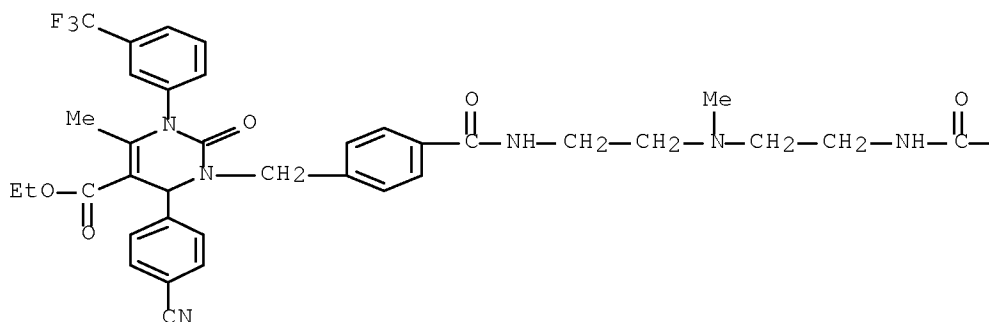
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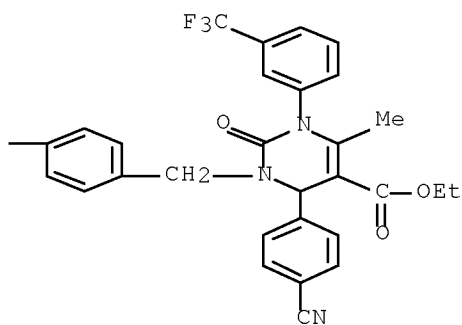
RN 904957-93-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[[4-[[[2-[[2-[[4-[[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]benzoyl]amino]ethyl]methylamino]ethyl]amino]carbonyl]phenyl]methyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

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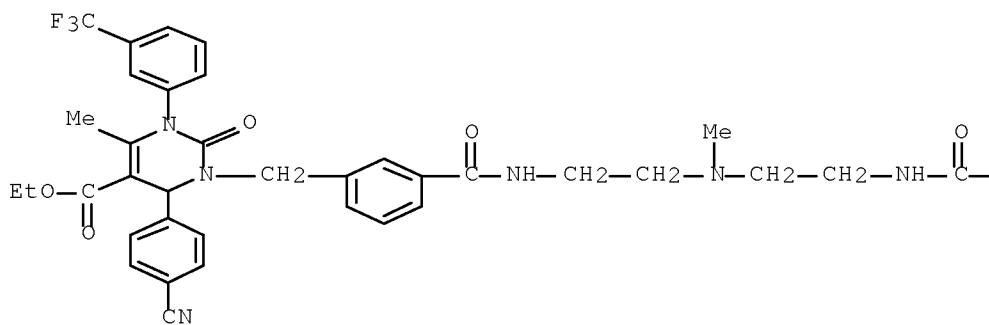
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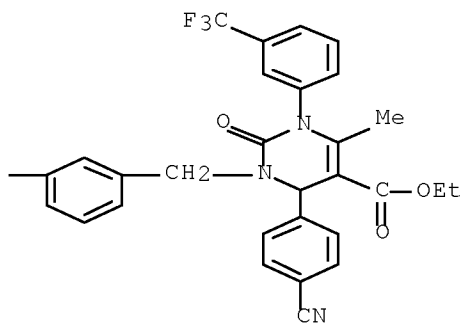
RN 904957-94-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[[3-[[[2-[[2-[[3-[[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]benzoyl]amino]ethyl]meth]ylamino]ethyl]amino]carbonyl]phenyl]methyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

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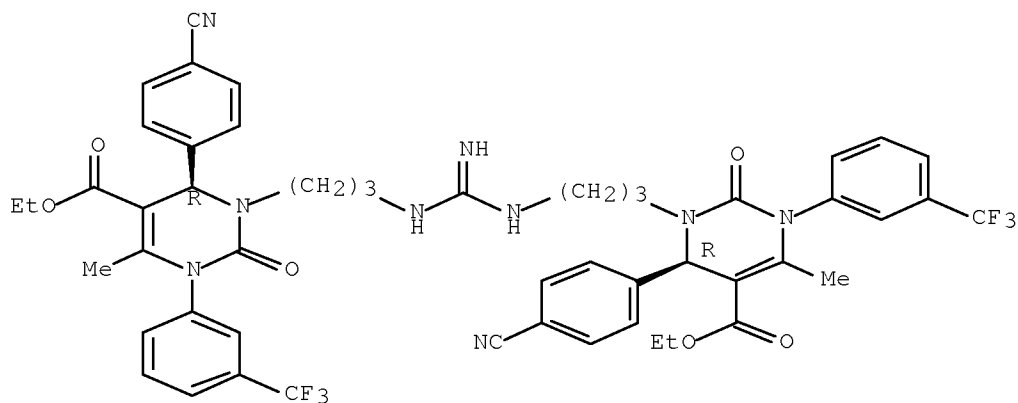
PAGE 1-B



RN 904957-95-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[carbonimidoylbis(imino-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

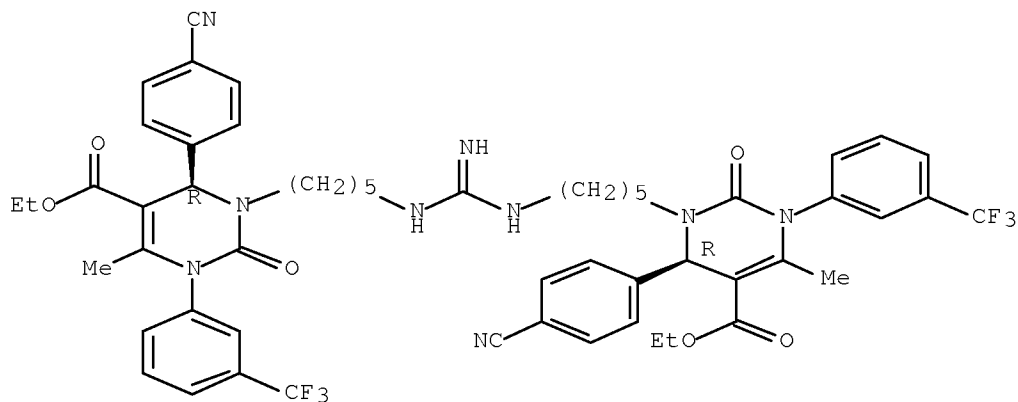
Absolute stereochemistry.



RN 904957-96-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[carbonimidoylbis(imino-5,1-pentanediy)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

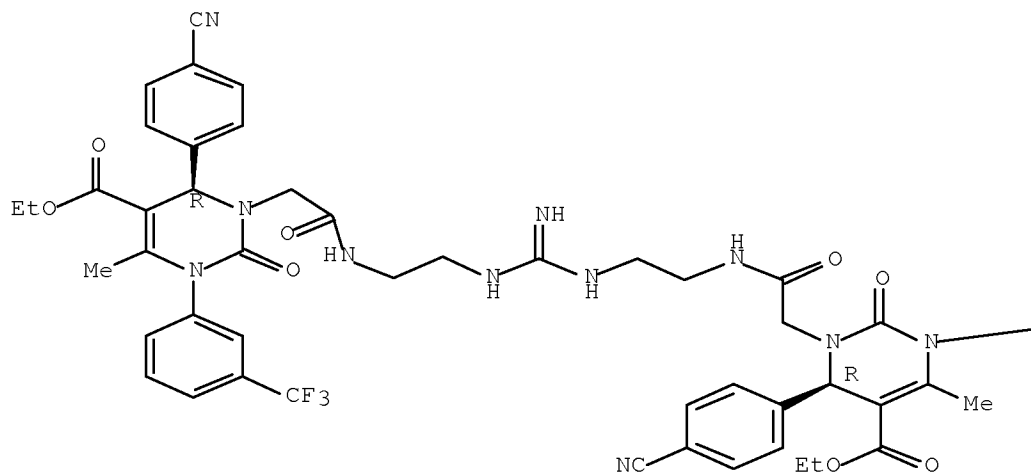


RN 904957-97-7 ZCAPLUS

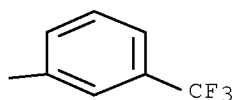
CN 5-Pyrimidinecarboxylic acid, 1,1'-(7-imino-2,12-dioxo-3,6,8,11-tetraaza-1,13-tridecanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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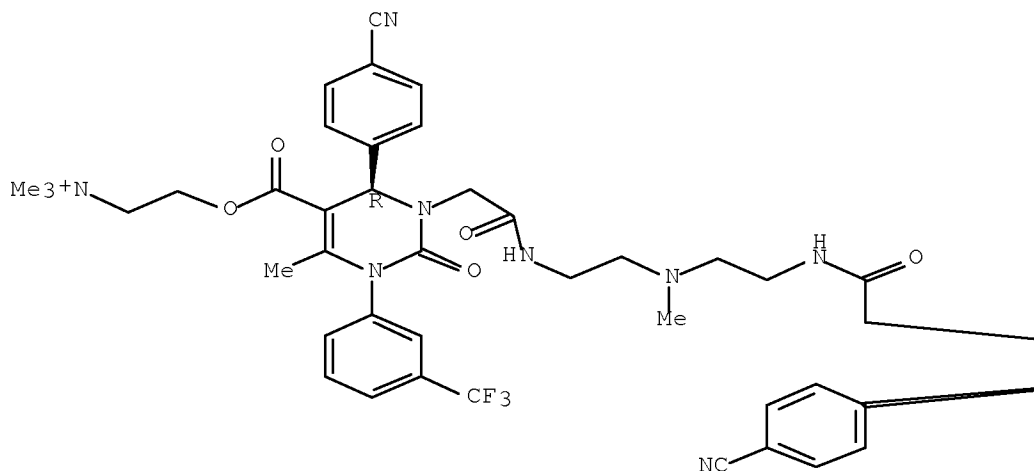


RN 904957-98-8 ZCAPLUS

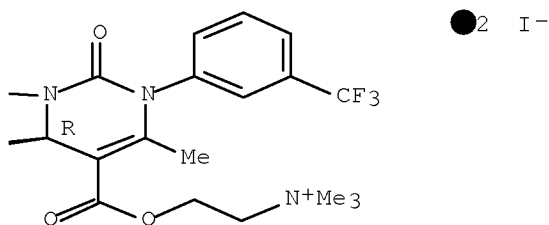
CN Ethanaminium, 2,2'-[(methylimino)bis[2,1-ethanediylimino(2-oxo-2,1-ethanediyl)] [(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1,5(2H)-pyrimidinediyl]carbonyloxy]]bis[N,N,N-trimethyl-, diiodide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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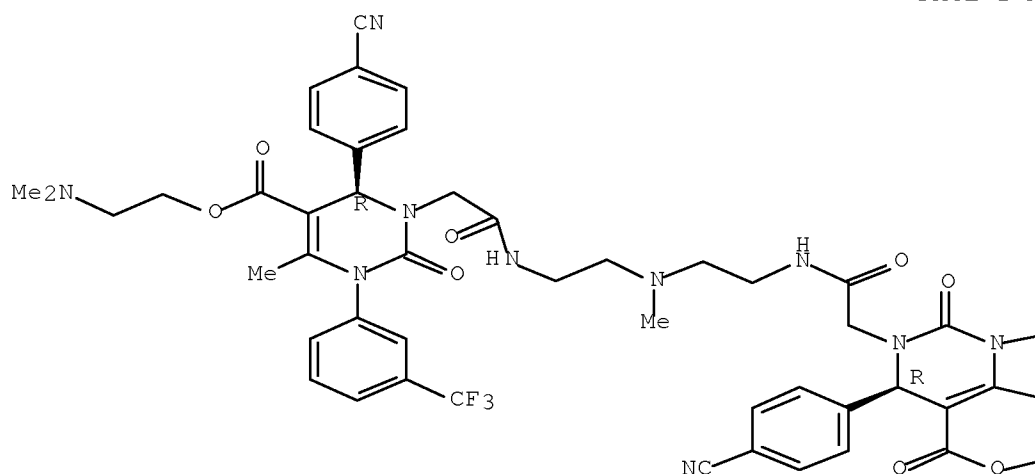


RN 904957-99-9 ZCAPLUS

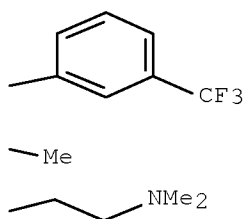
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-[[2-[[2-[(6R)-6-(4-cyanophenyl)-5-[[2-(dimethylamino)ethoxy]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(dimethylamino)ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

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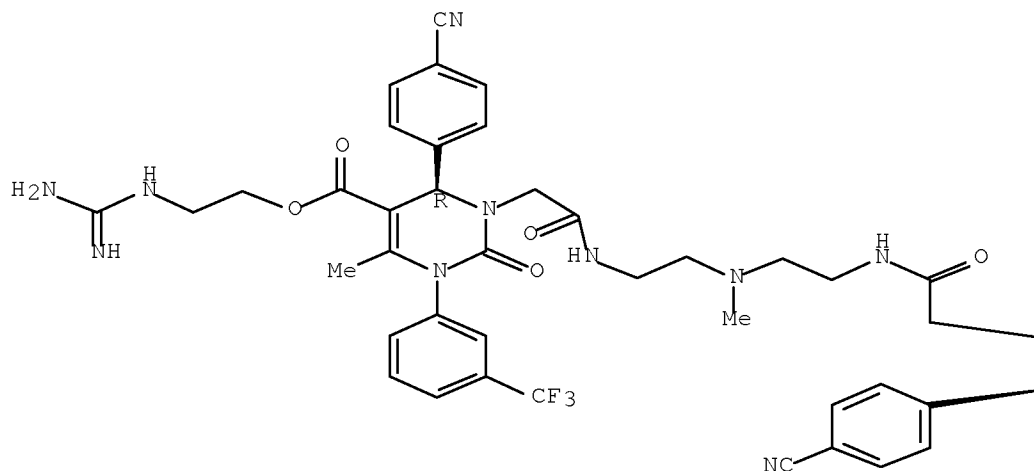


RN 904958-00-5 ZCAPLUS

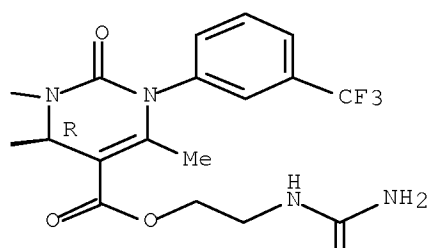
CN 5-Pyrimidinecarboxylic acid, 3-[2-[[2-[[2-[[2-[(6R)-5-[[2-
[(aminoiminomethyl)amino]ethoxy]carbonyl]-6-(4-cyanophenyl)-3,6-dihydro-4-
methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-
pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-4-(4-
cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-
(trifluoromethyl)phenyl]-, 2-[(aminoiminomethyl)amino]ethyl ester, (4R)-
(CA INDEX NAME)

Absolute stereochemistry.

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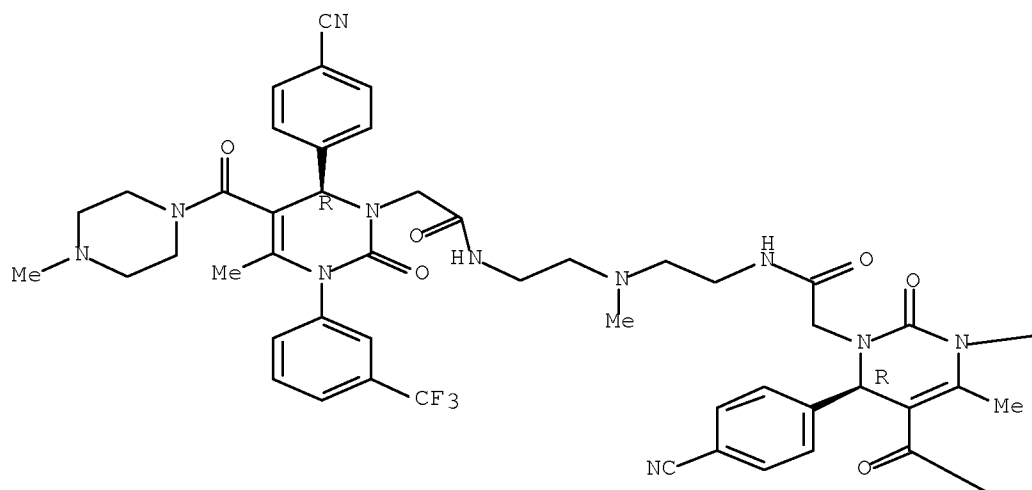


RN 904958-01-6 ZCAPLUS

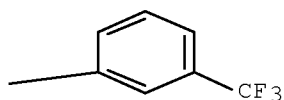
CN 1(2H)-Pyrimidineacetamide, N,N'-[(methylimino)di-2,1-ethanediyl]bis[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-[(4-methyl-1-piperazinyl)carbonyl]-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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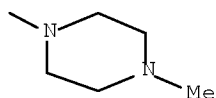


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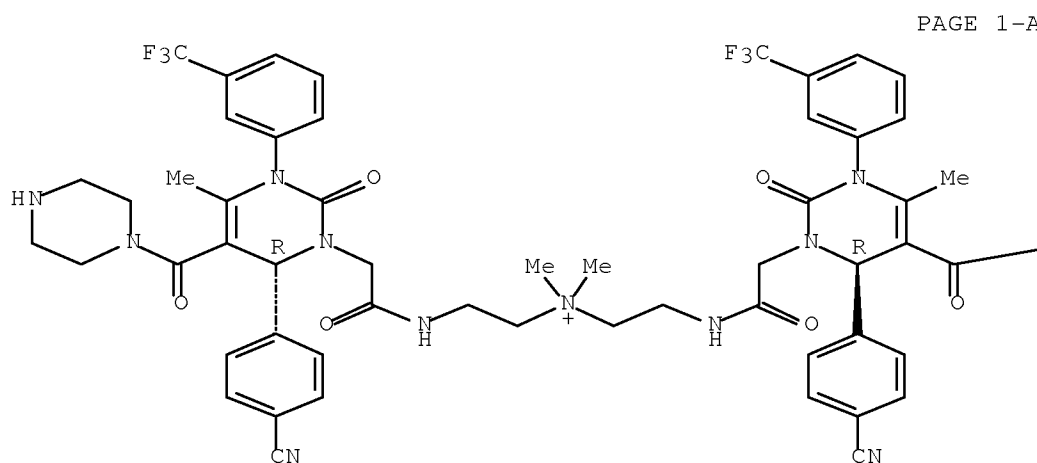
RN 904958-02-7 ZCAPLUS
 CN 1(2H)-Pyrimidineacetamide, N,N'-[(methylimino)di-2,1-ethanediyl]bis[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(1-piperazinylcarbonyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R,6'R)- (9CI) (CA INDEX NAME)

The chemical structure shows a complex molecule with two pyrimidine rings connected by a long chain. The left pyrimidine ring is substituted with a cyano group (CN) at the 2-position and a trifluoromethyl group (CF₃) at the 6-position. It is linked via a carbonyl group to a piperidine ring. The right pyrimidine ring is substituted with a cyano group (NC) at the 2-position and a methyl group (Me) at the 6-position. It is linked via a carbonyl group to a secondary amine chain. The chain includes a piperidine ring, a carbonyl group, and a secondary amine.

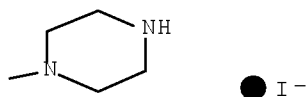
CN1CCCC1

51

Absolute stereochemistry.



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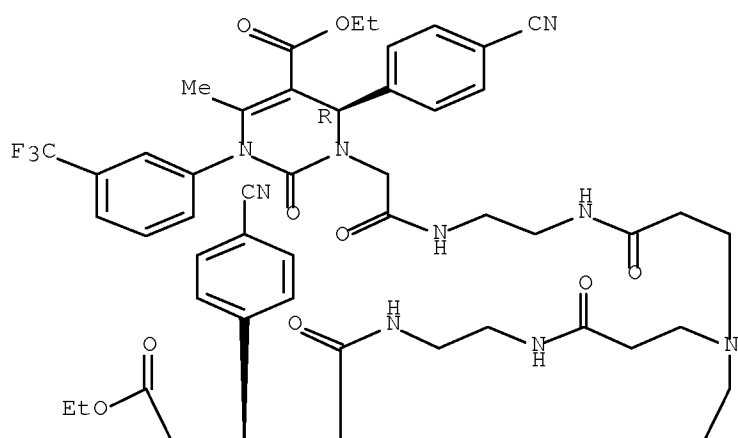


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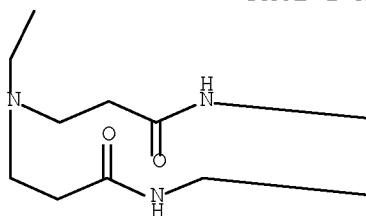
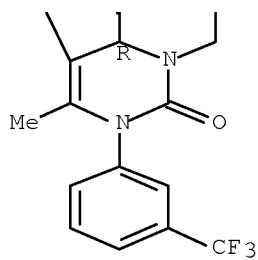
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[22-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]-10,13-bis[3-[[2-[[2-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]amino]-3-oxopropyl]-2,7,16,21-tetraoxo-3,6,10,13,17,20-hexaazadocos-1-yl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

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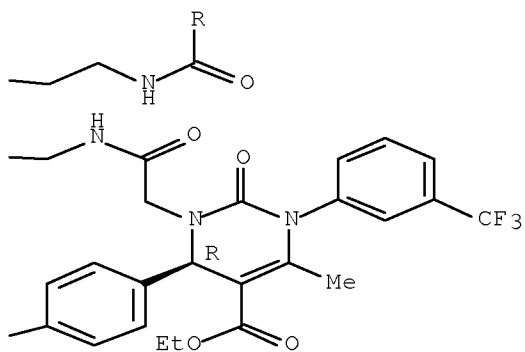


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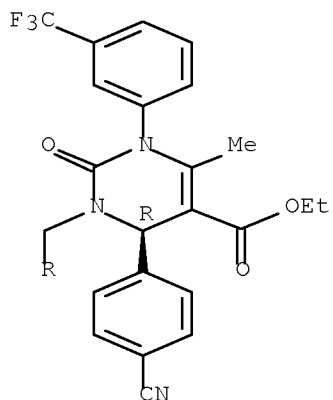


NC

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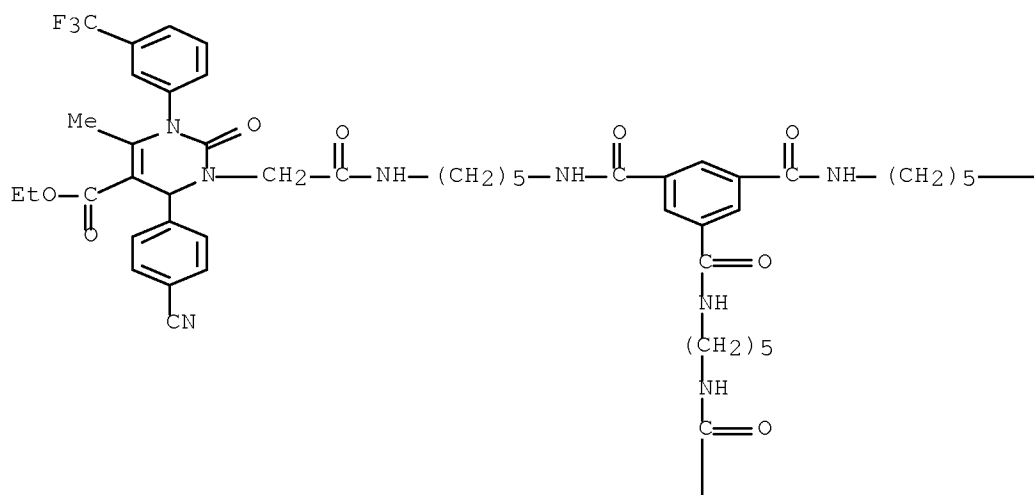
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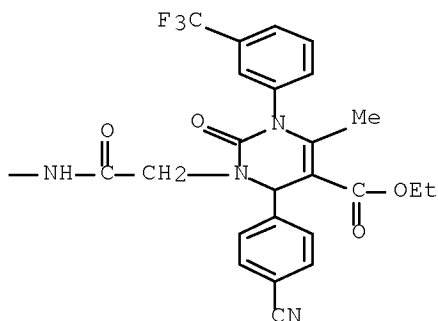
RN 904958-05-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[2-[[5-[[3,5-bis[[[5-[[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]pentyl]amino]carbo-
nyl]benzoyl]amino]pentyl]amino]-2-oxoethyl]-4-(4-cyanophenyl)-1,2,3,4-
tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA
INDEX NAME)

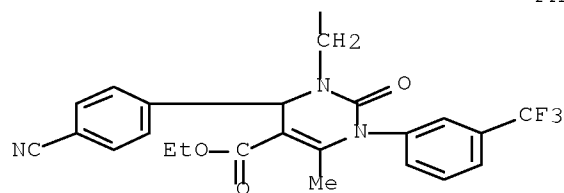
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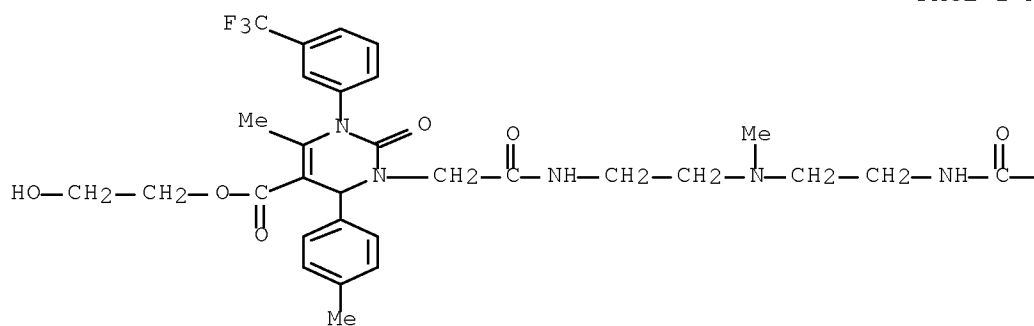
PAGE 2-A



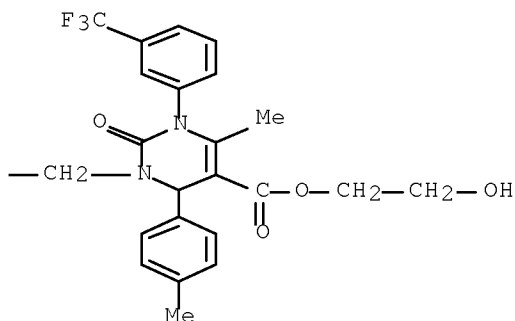
RN 904958-06-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[2-[[2-[[2-[[2-[3,6-dihydro-5-[(2-hydroxyethoxy)carbonyl]-4-methyl-6-(4-methylphenyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-4-(4-methylphenyl)-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-hydroxyethyl ester (CA INDEX NAME)

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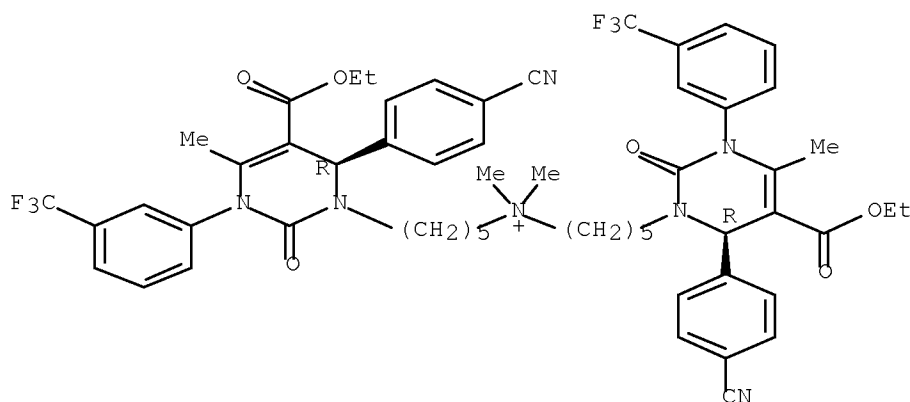


RN 904958-08-3 ZCAPLUS

CN 1(2H)-Pyrimidinepentanaminium, 6-(4-cyanophenyl)-N-[5-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]pentyl]-5-(ethoxycarbonyl)-3,6-dihydro-N,N,4-trimethyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, iodide (1:1), (6R)- (CA INDEX NAME)

Absolute stereochemistry.

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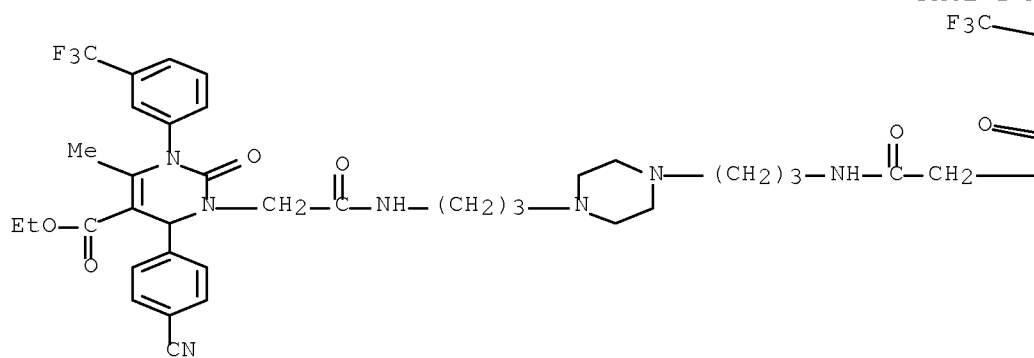
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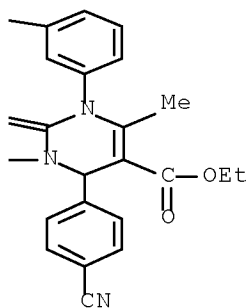
RN 904958-09-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[3-[4-[3-[[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]propyl]-1-piperazinyl]propyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

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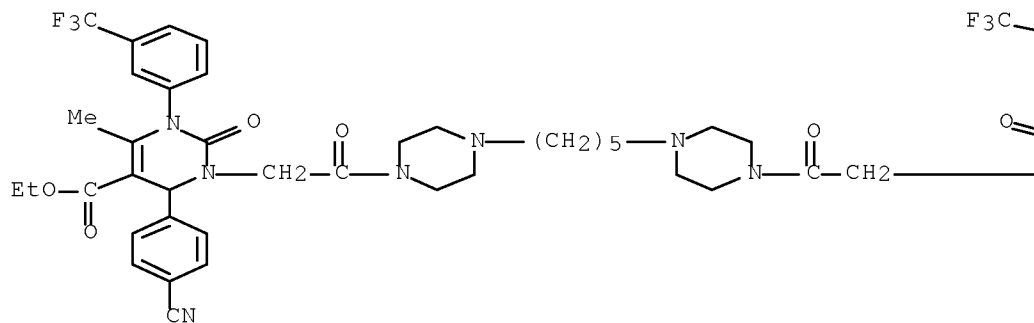
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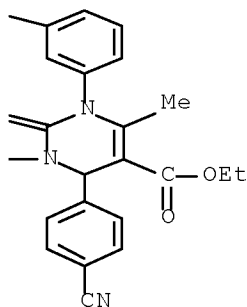
RN 904958-10-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[5-[4-[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]pentyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

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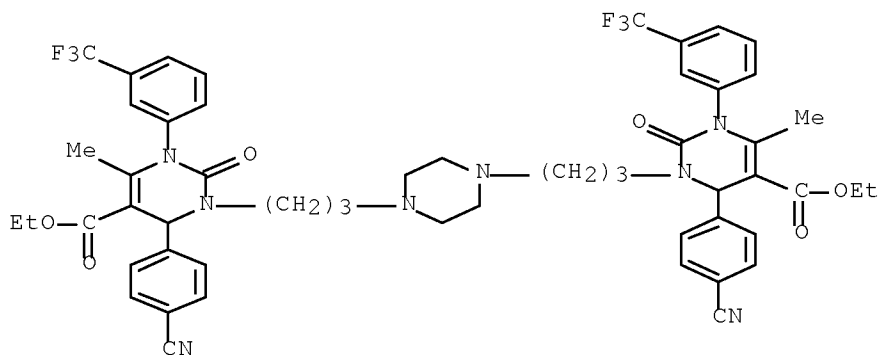


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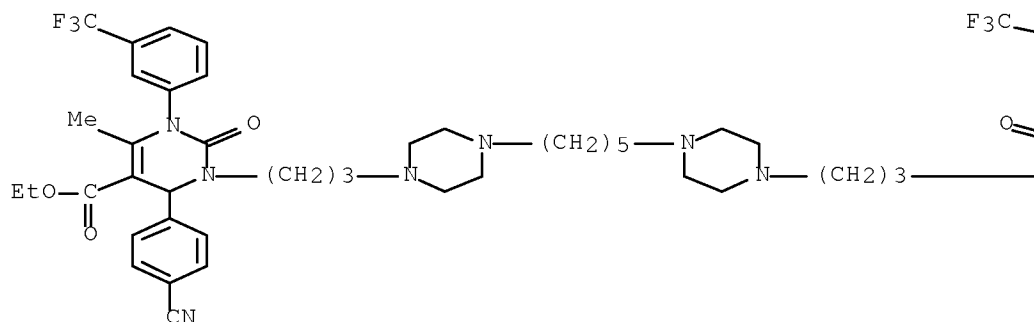
RN 904958-11-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,4-piperazinediyl)di-3,1-propanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 904958-12-9 ZCAPLUS

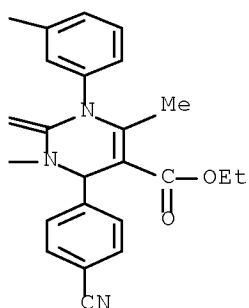
CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,5-pentanediy]bis(4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



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F₃C

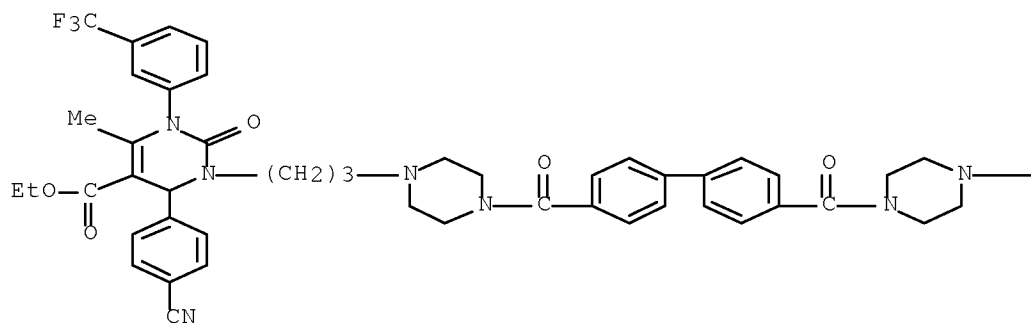
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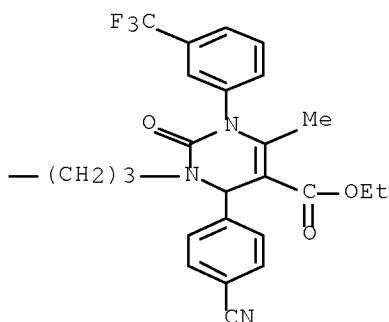
RN 904958-13-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[[1,1'-biphenyl]-4,4'-diylbis(carbonyl-4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

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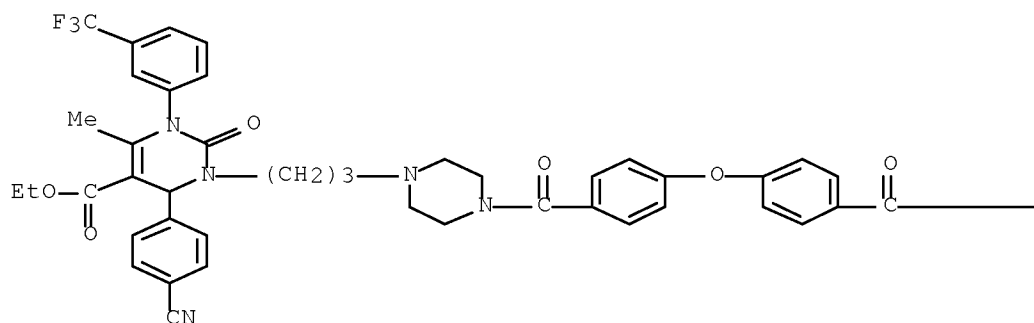
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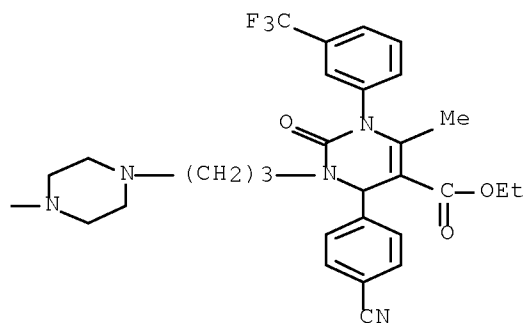
RN 904958-14-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[oxybis(4,1-phenylenecarbonyl-4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

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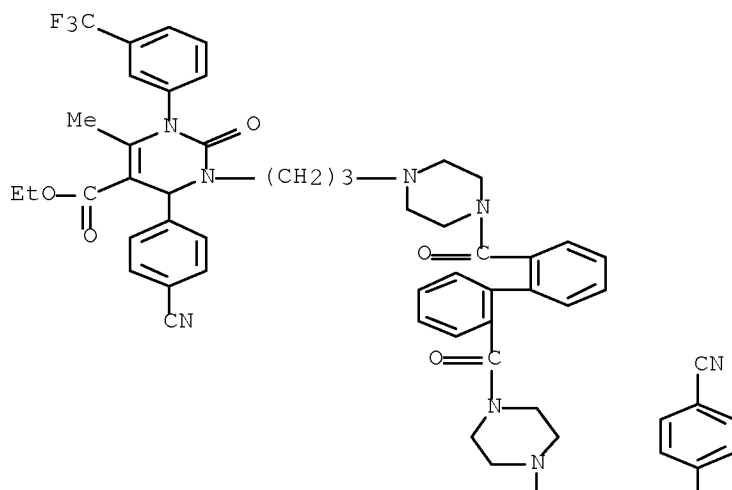
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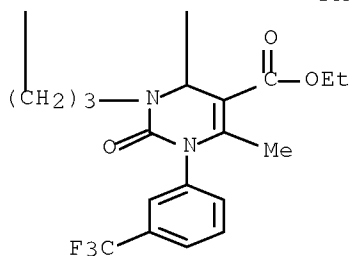
RN 904958-15-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[[1,1'-biphenyl]-2,2'-diylbis(carbonyl-4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

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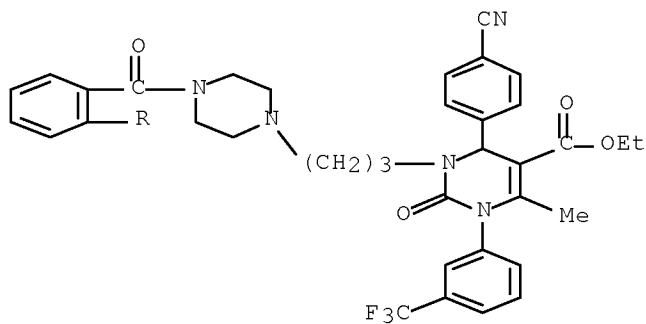


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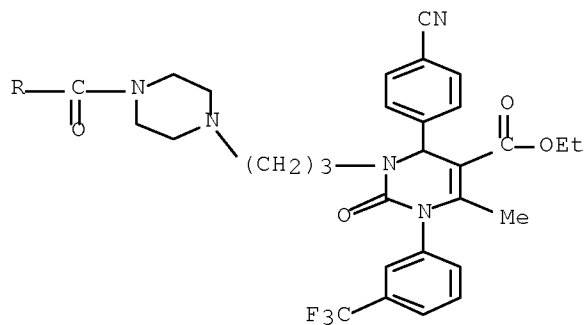


RN 904958-16-3 ZCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,2-phenylenebis(carbonyl-4,1-piperazinediyl)-3,1-propanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

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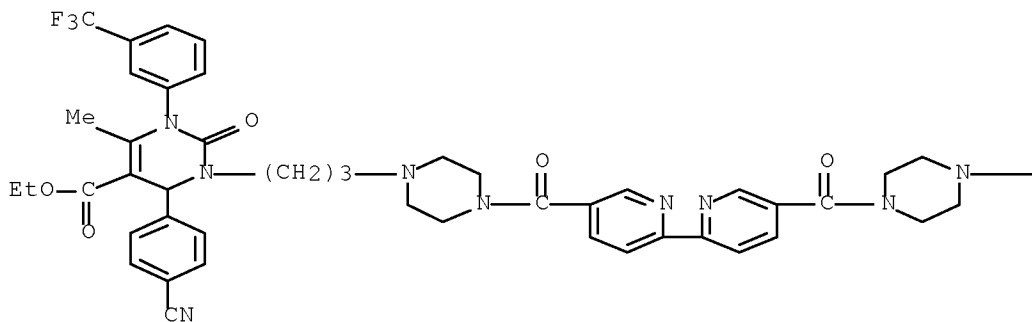


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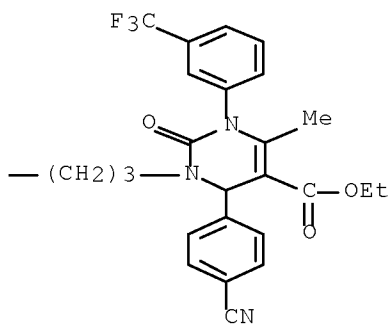


RN 904958-17-4 ZCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 1,1'-[[2,2'-bipyridin]-5,5'-diylbis(carbonyl-4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

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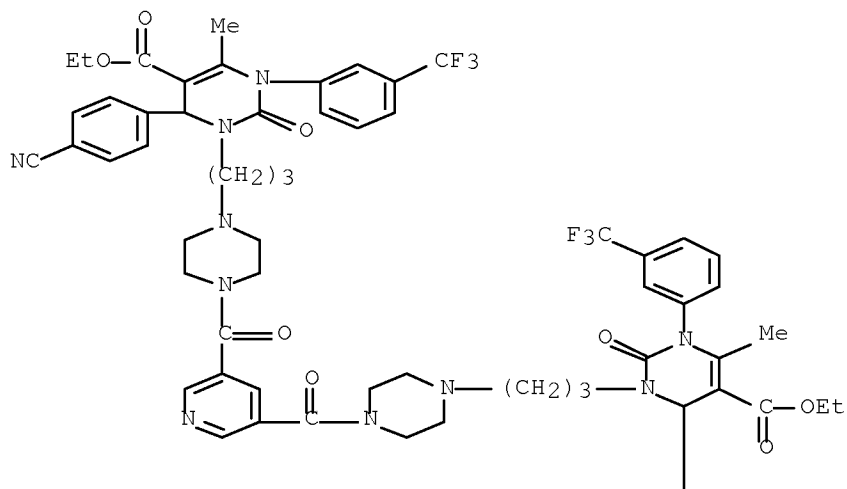


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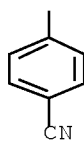


RN 904958-18-5 ZCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 1,1'-[3,5-pyridinediylbis(carbonyl-4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

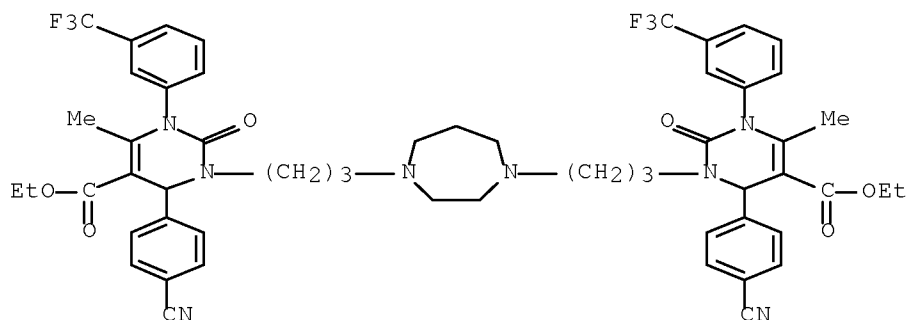
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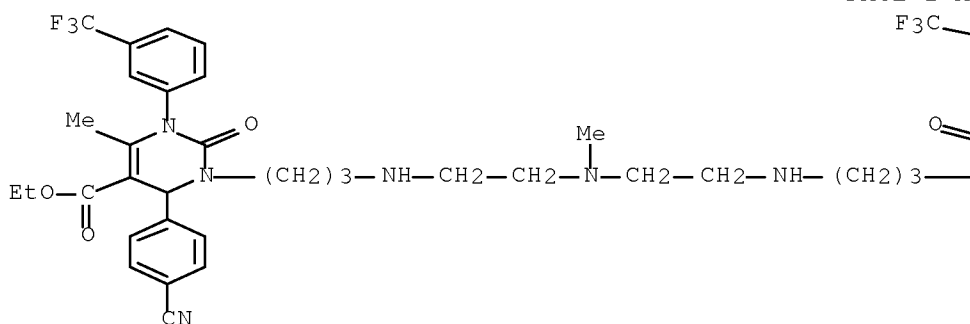


RN 904958-19-6 ZCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 1,1'-[(tetrahydro-1H-1,4-diazepine-1,4(5H)-diyl)di-3,1-propanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

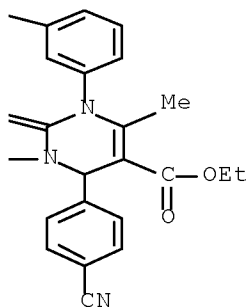


RN 904958-20-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[(methylimino)bis(2,1-ethanediylimino-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

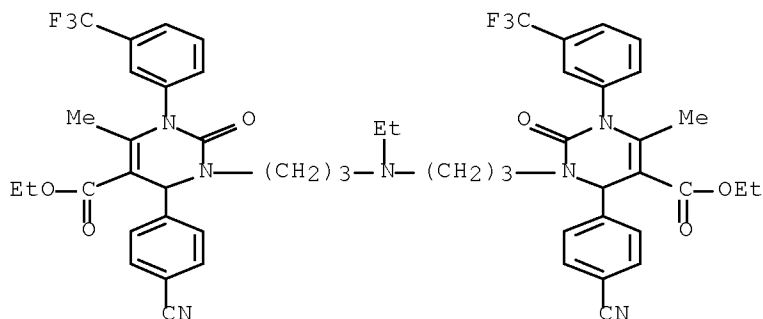


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RN 904958-21-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[(ethylimino)di-2,1-ethanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

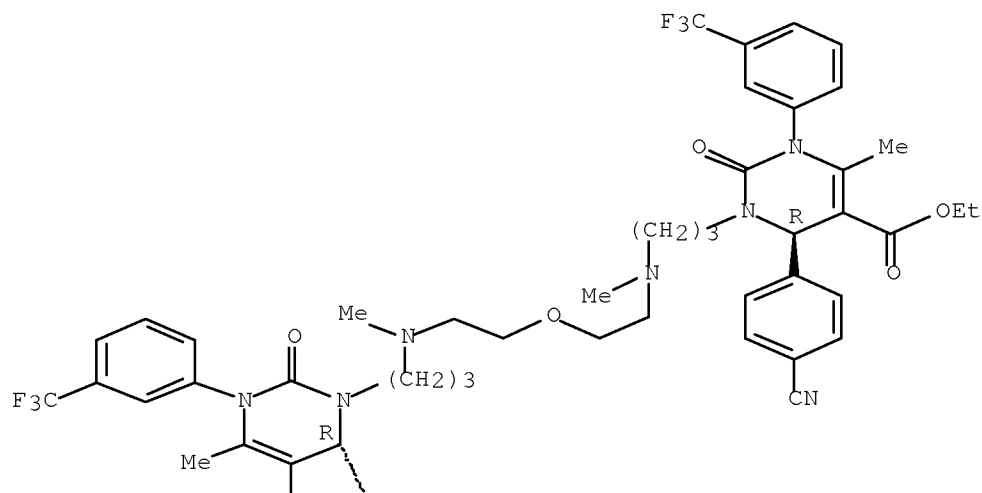


RN 904958-22-1 ZCAPLUS

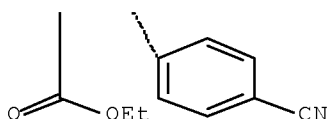
CN 5-Pyrimidinecarboxylic acid, 1,1'-[oxybis[2,1-ethanediyl(methylimino)-3,1-propanediyl]]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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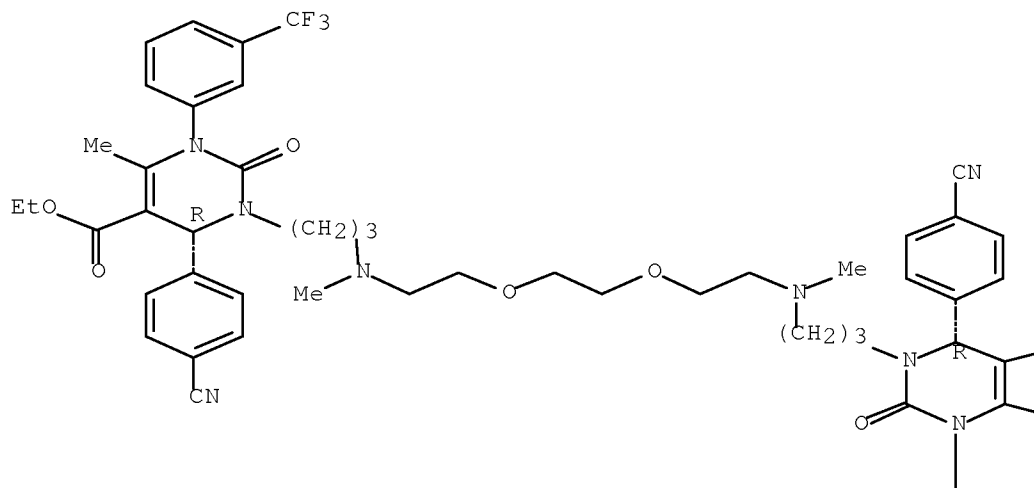


RN 904958-23-2 ZCAPLUS

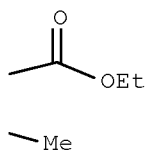
CN 5-Pyrimidinecarboxylic acid, 1,1'-(4,13-dimethyl-7,10-dioxa-4,13-diazahexadecane-1,16-diyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

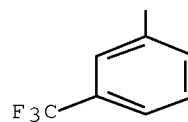
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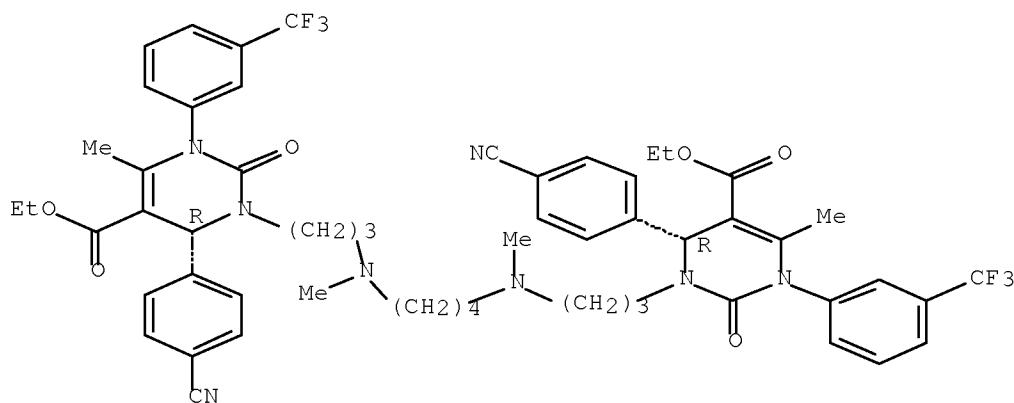


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RN 904958-24-3 ZCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,4-butanediylbis[(methylimino)-3,1-propanediyl]]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

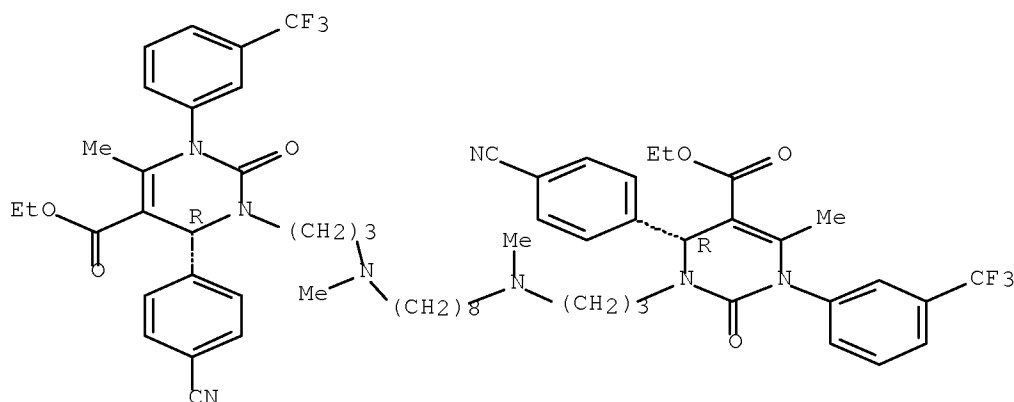
Absolute stereochemistry.



RN 904958-25-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,8-octanediylbis[(methylimino)-3,1-propanediyl]]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

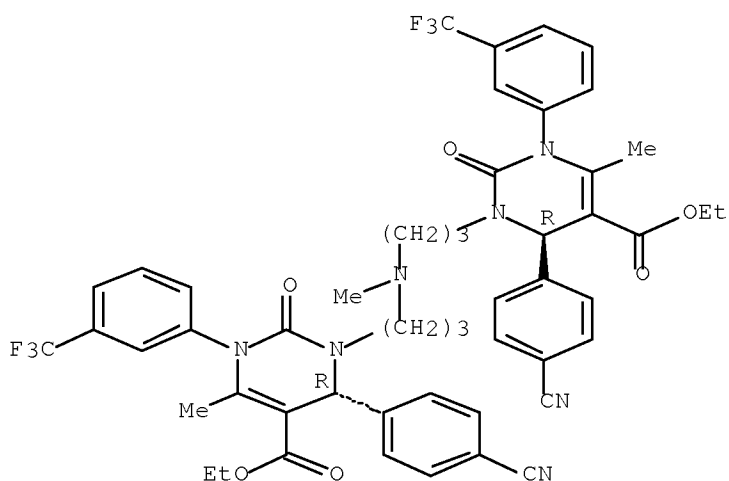
Absolute stereochemistry.



RN 904958-26-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[(methylimino)di-2,1-ethanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

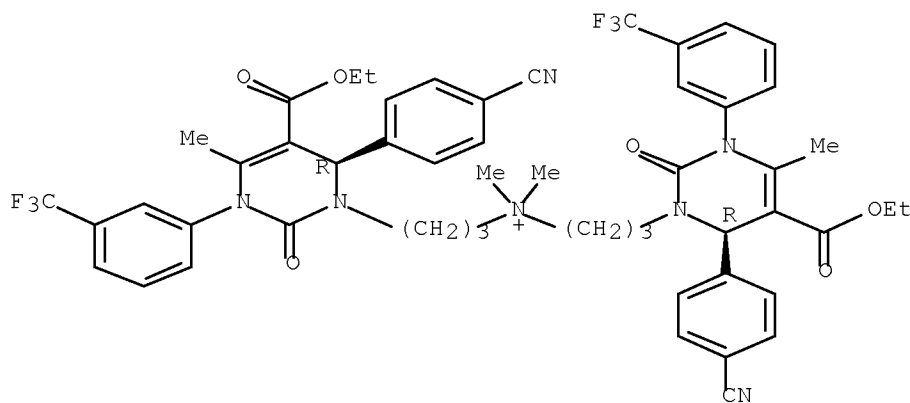


RN 904958-27-6 ZCAPLUS

CN 1(2H)-Pyrimidinepropanaminium, 6-(4-cyanophenyl)-N-[3-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-5-(ethoxycarbonyl)-3,6-dihydro-N,N,4-trimethyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, iodide (1:1), (6R)- (CA INDEX NAME)

Absolute stereochemistry.

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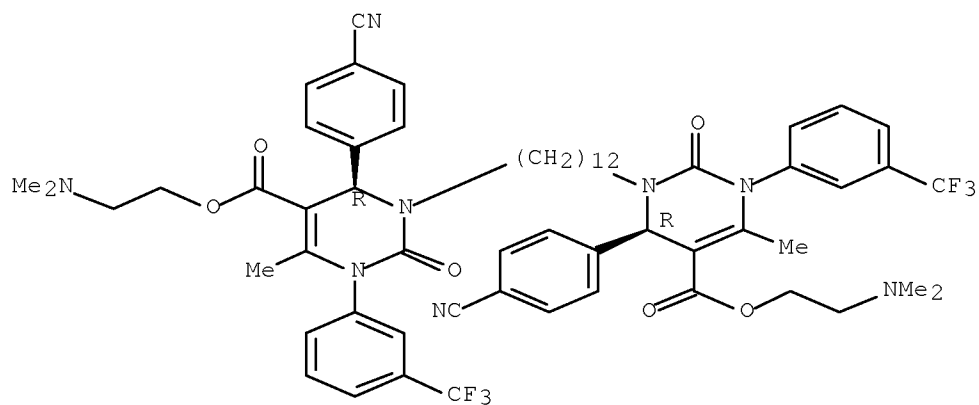
PAGE 2-A

● I⁻

RN 904958-28-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,12-dodecanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis[2-(dimethylamino)ethyl] ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 904958-30-1 ZCAPLUS

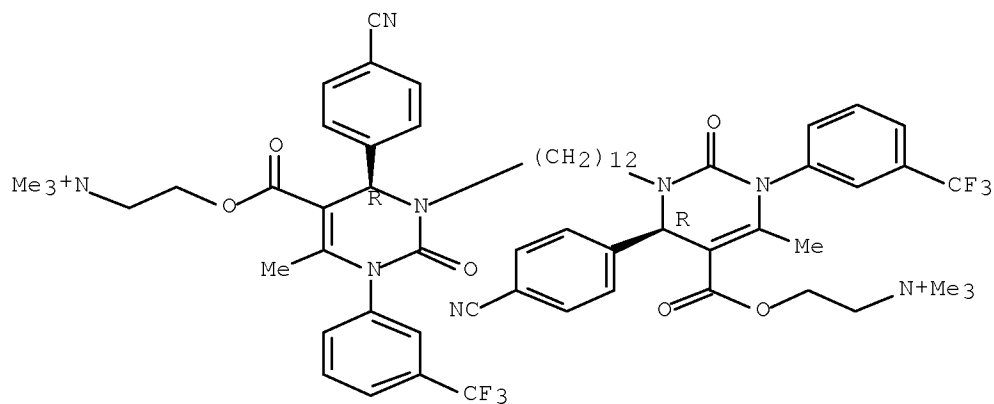
CN Ethanaminium, 2-[[[(4R)-4-(4-cyanophenyl)-3-[12-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-5-[[2-(trimethylammonio)ethoxy]carbonyl]-1(2H)-pyrimidinyl]dodecyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]oxy]-N,N,N-trimethyl-, formate (1:2) (CA INDEX NAME)

CM 1

CRN 904958-29-8

CMF C62 H74 F6 N8 O6

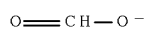
Absolute stereochemistry.



CM 2

CRN 71-47-6

CMF C H O2

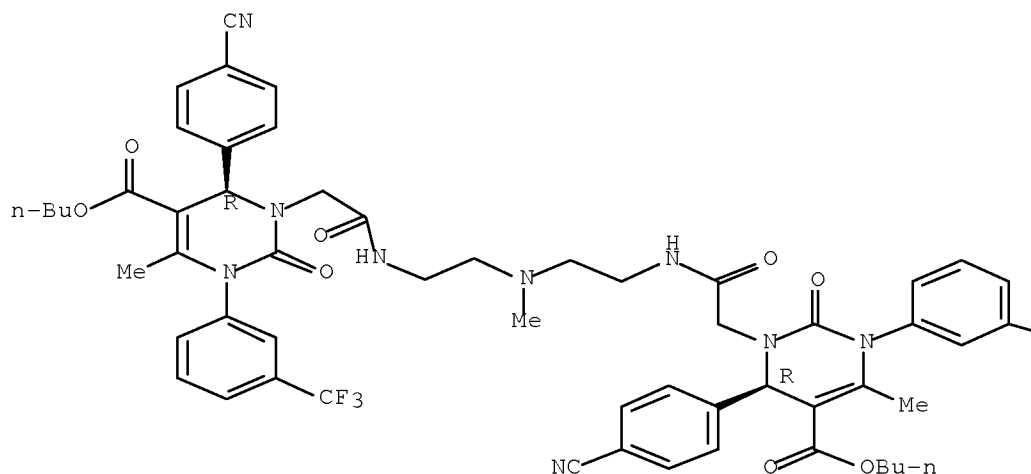


RN 904958-31-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[2-[[2-[[2-[[2-[(6R)-5-(butoxycarbonyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, butyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

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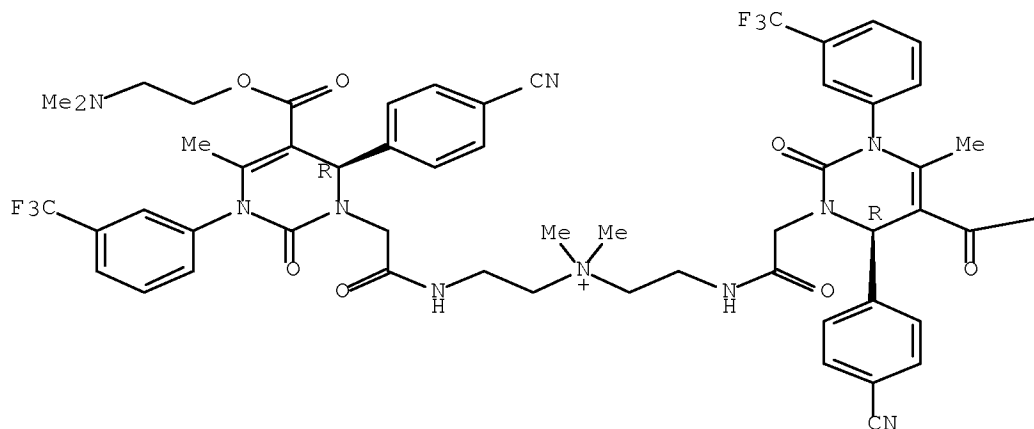
—CF₃

RN 904958-32-3 ZCAPLUS

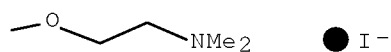
CN Ethanaminium, 2-[[2-[(6R)-6-(4-cyanophenyl)-5-[[2-(dimethylamino)ethoxy]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[(6R)-6-(4-cyanophenyl)-5-[[2-(dimethylamino)ethoxy]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

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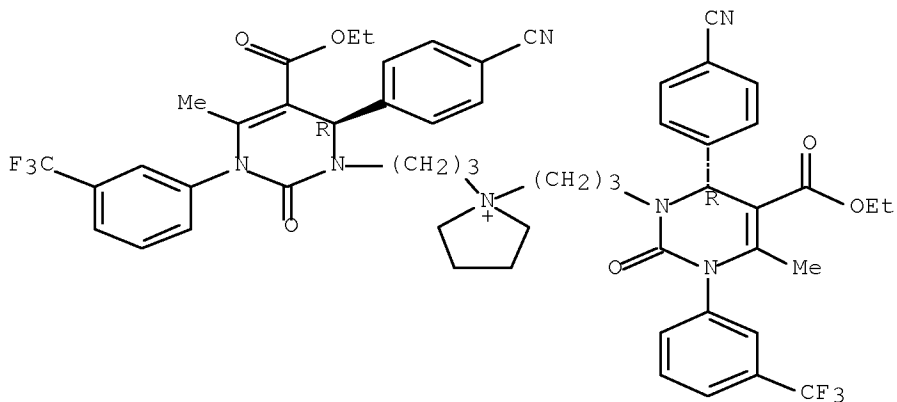


RN 904958-33-4 ZCAPLUS

CN Pyrrolidinium, 1,1-bis[3-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

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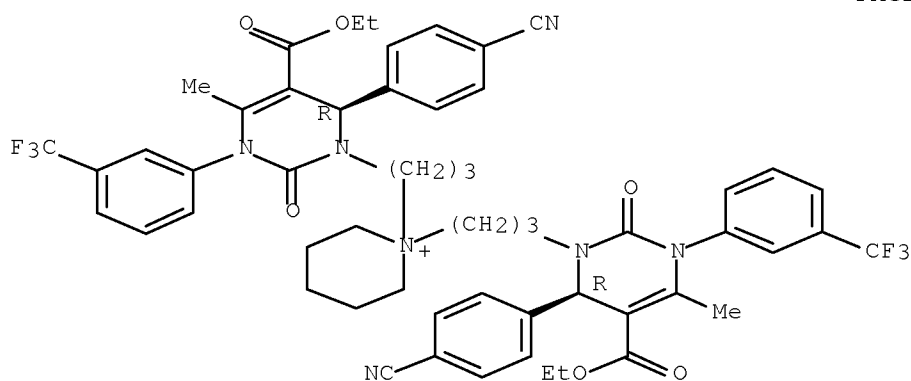


RN 904958-34-5 ZCAPLUS

CN Piperidinium, 1,1-bis[3-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

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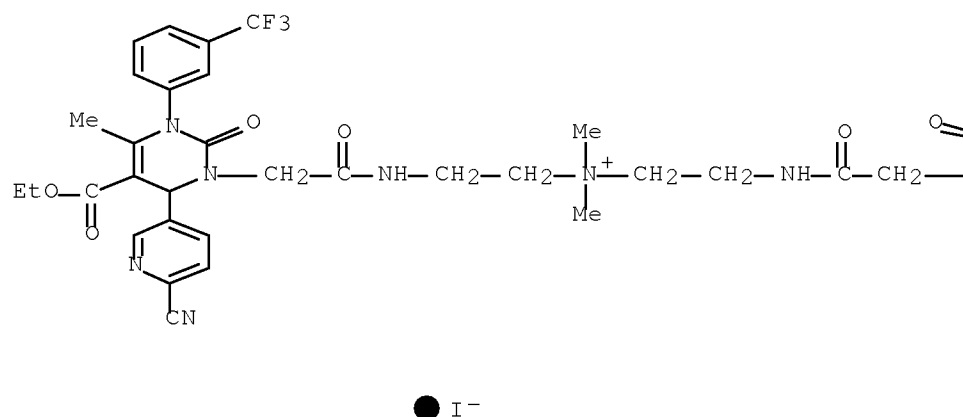
PAGE 2-A



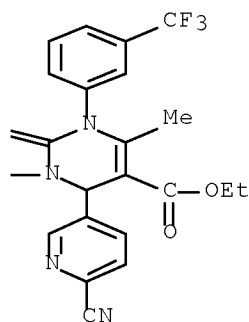
RN 904958-36-7 ZCAPLUS

CN Ethanaminium, 2-[[2-[6-(6-cyano-3-pyridinyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[6-(6-cyano-3-pyridinyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

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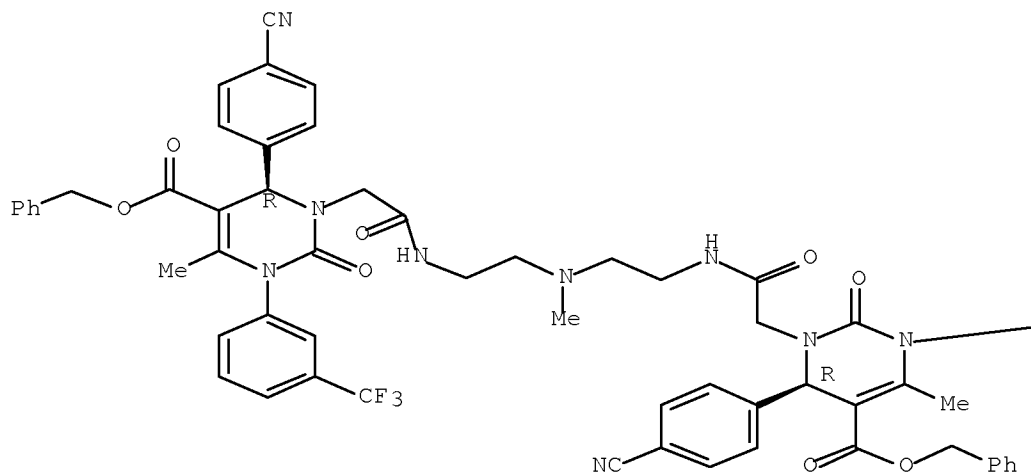


RN 904958-37-8 ZCAPLUS

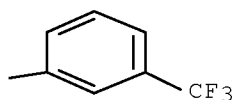
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-[[2-[[2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(phenylmethoxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, phenylmethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

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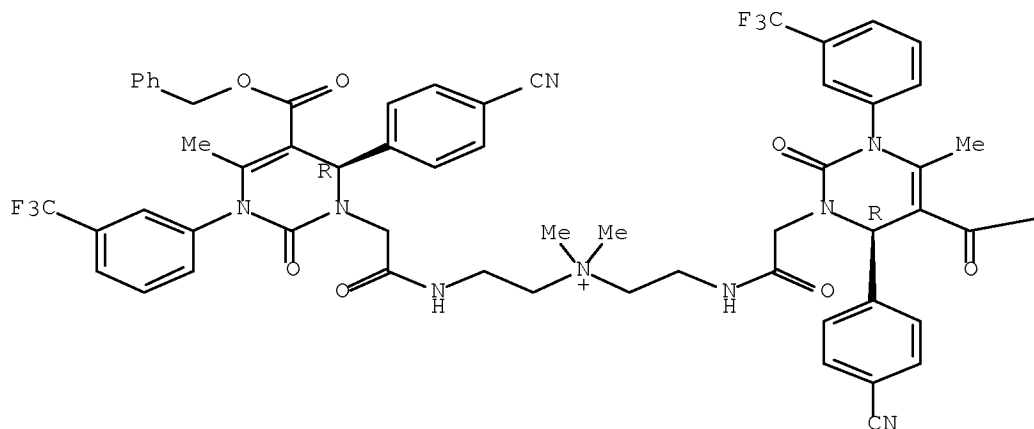
RN 904958-39-0 ZCAPLUS
 CN Ethanaminium, 2-[[2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(phenylmethoxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(phenylmethoxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, formate (1:1) (CA INDEX NAME)

CM 1

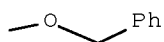
CRN 904958-38-9
 CMF C64 H58 F6 N9 O8

Absolute stereochemistry.

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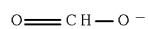
PAGE 1-B



CM 2

CRN 71-47-6

CMF C H O2



RN 904958-41-4 ZCAPLUS

CN Ethanaminium, 2-[[[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, butanedioate (2:1) (9CI) (CA INDEX NAME)

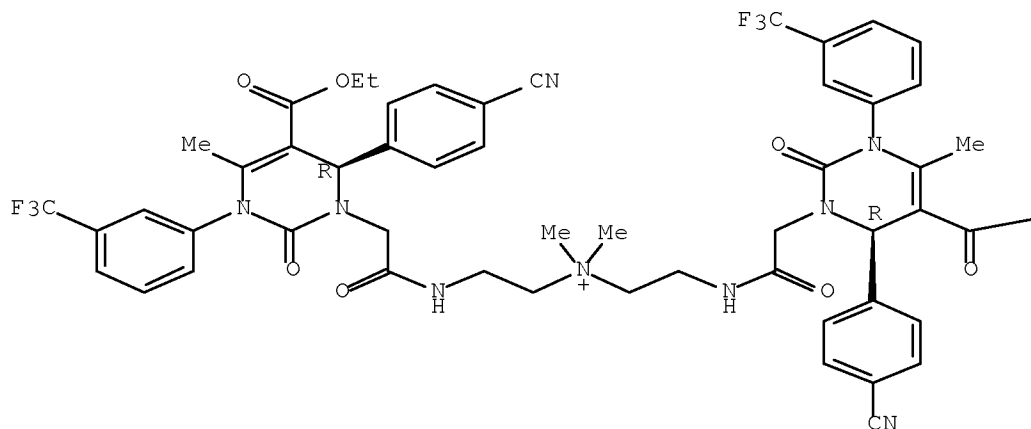
CM 1

CRN 904958-40-3

CMF C54 H54 F6 N9 O8

Absolute stereochemistry.

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—OEt

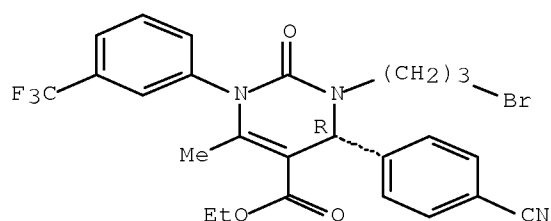
CM 2

CRN 56-14-4
CMF C4 H4 O4

—O₂C—CH₂—CH₂—CO₂—

IT 904958-45-8P
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of multimers of tetrahydropyrimidinone compds.)
as elastase inhibitors useful in the treatment of respiratory diseases)
RN 904958-45-8 ZCAPLUS
CN 5-Pyrimidinecarboxylic acid, 3-(3-bromopropyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.



IT 904958-43-6P 904958-44-7P 904958-46-9P
 904958-47-0P 904958-48-1P 904958-49-2P
 904958-51-6P 904958-52-7P 904958-53-8P
 904958-54-9P 904958-55-0P 904958-56-1P
 904958-57-2P 904958-58-3P 904958-59-4P
 904958-60-7P 904958-61-8P 904958-62-9P
 904958-63-0P 904958-64-1P 904958-65-2P
 904958-66-3P 904958-67-4P 904958-68-5P
 904958-69-6P 904958-70-9P 904958-71-0P
 904958-72-1P 904958-75-4P 904958-76-5P
 904958-77-6P 904958-79-8P 904958-80-1P
 904958-81-2P 904958-83-4P 904958-97-0P
 904958-98-1P 904958-99-2P 904959-00-8P
 904959-03-1P 904959-04-2P 904959-05-3P
 904959-06-4P 904959-08-6P 904959-16-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(intermediate; preparation of multimers of tetrahydropyrimidinone compds.

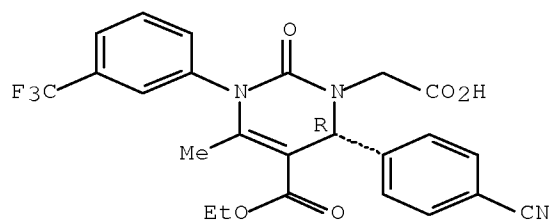
as

elastase inhibitors useful in the treatment of respiratory diseases)

RN 904958-43-6 ZCAPLUS

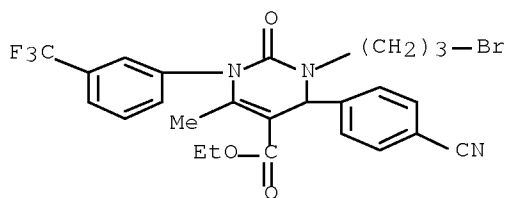
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-
 dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX
 NAME)

Absolute stereochemistry.



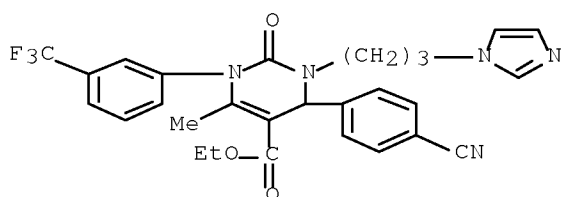
RN 904958-44-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(3-bromopropyl)-4-(4-cyanophenyl)-1,2,3,4-
 tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA
 INDEX NAME)



RN 904958-46-9 ZCAPLUS

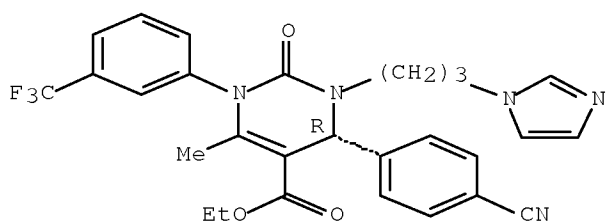
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[3-(1H-imidazol-1-yl)propyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-47-0 ZCAPLUS

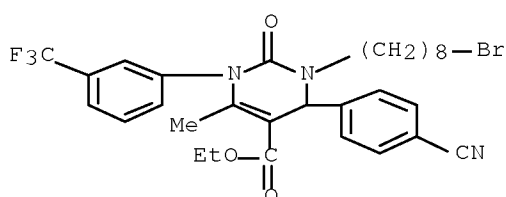
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[3-(1H-imidazol-1-yl)propyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 904958-48-1 ZCAPLUS

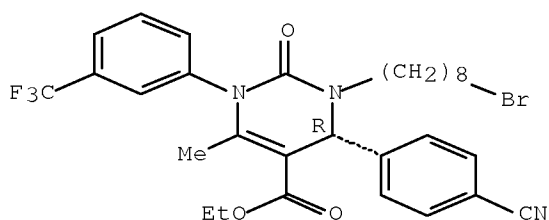
CN 5-Pyrimidinecarboxylic acid, 3-(8-bromooctyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-49-2 ZCAPLUS

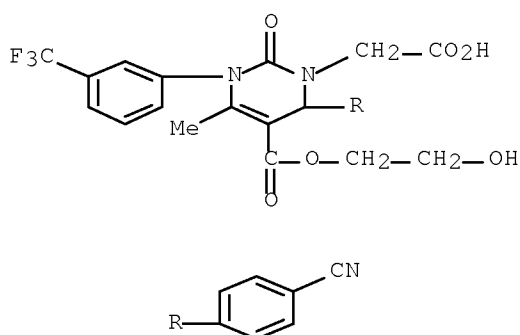
CN 5-Pyrimidinecarboxylic acid, 3-(8-bromooctyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 904958-51-6 ZCAPLUS

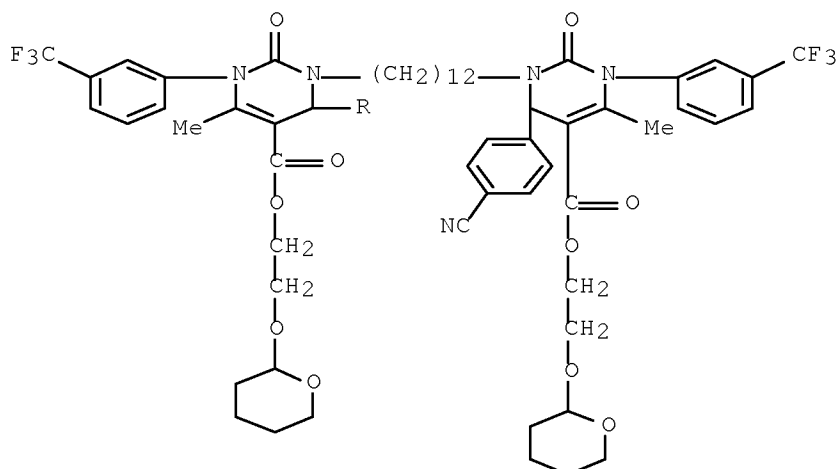
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-5-[(2-hydroxyethoxy)carbonyl]-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



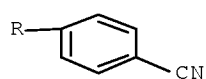
RN 904958-52-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,12-dodecanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis[2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl] ester (9CI) (CA INDEX NAME)

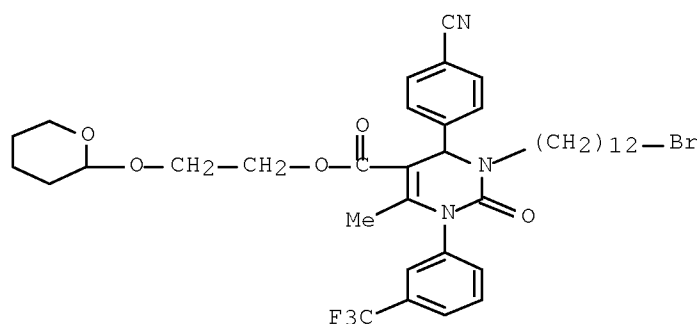
PAGE 1-A



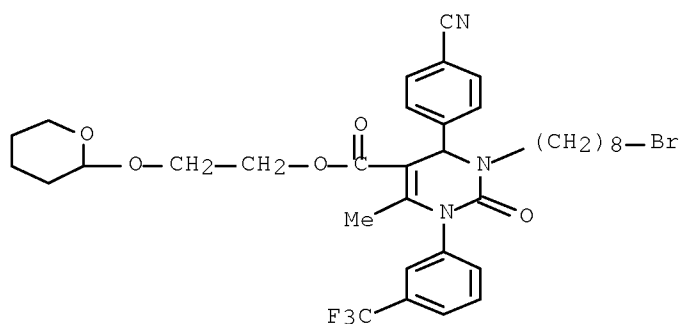
PAGE 2-A



RN 904958-53-8 ZCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 3-(12-bromododecyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl ester (CA INDEX NAME)

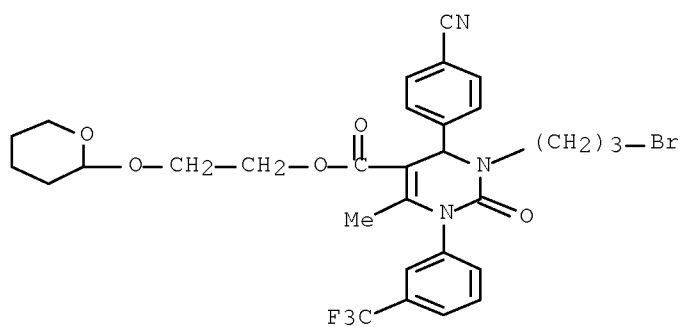


RN 904958-54-9 ZCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 3-(8-bromooctyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl ester (CA INDEX NAME)



RN 904958-55-0 ZCAPLUS

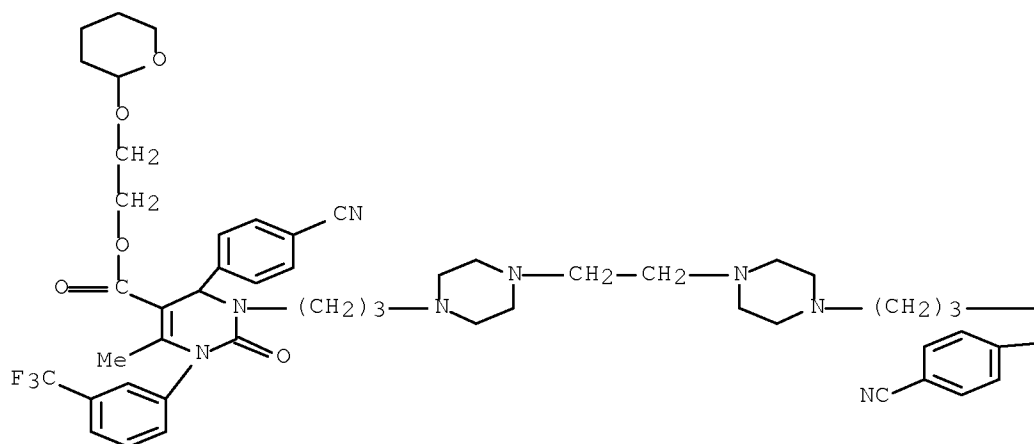
CN 5-Pyrimidinecarboxylic acid, 3-(3-bromopropyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl ester (CA INDEX NAME)



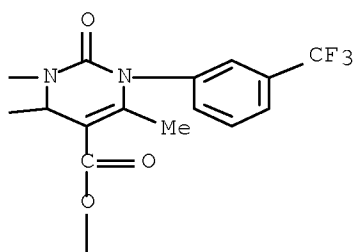
RN 904958-56-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,2-ethanediylbis(4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis[2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl] ester (9CI) (CA INDEX NAME)

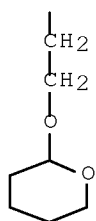
PAGE 1-A



PAGE 1-B

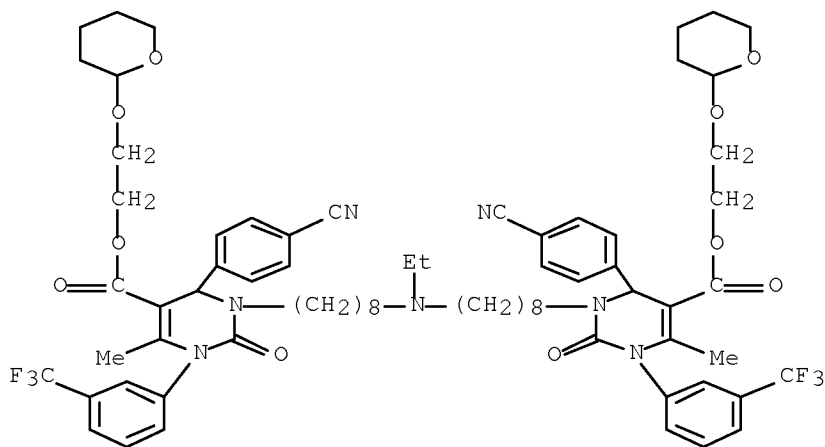


PAGE 2-B



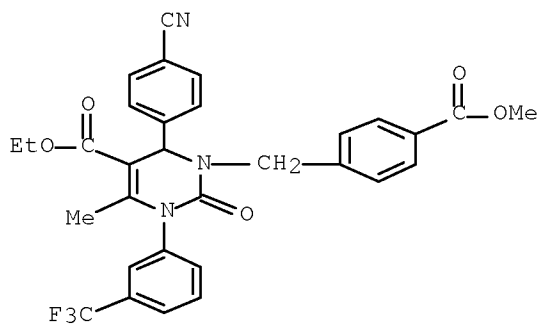
RN 904958-57-2 ZCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 1,1'-[(ethylimino)di-8,1-octanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-

(trifluoromethyl)phenyl]-, bis[2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl]
ester (9CI) (CA INDEX NAME)



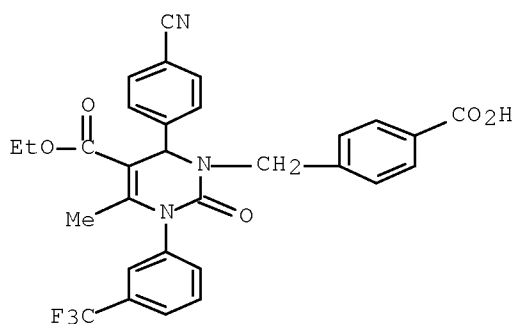
RN 904958-58-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[[4-(methoxycarbonyl)phenyl]methyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



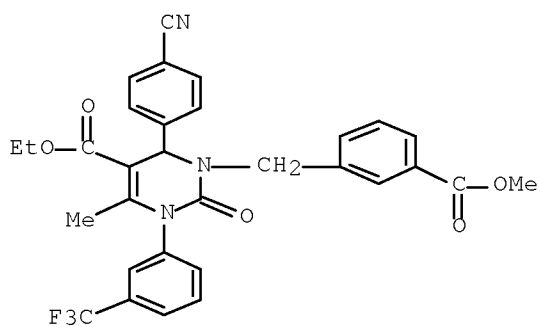
RN 904958-59-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[(4-carboxyphenyl)methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 5-ethyl ester (CA INDEX NAME)



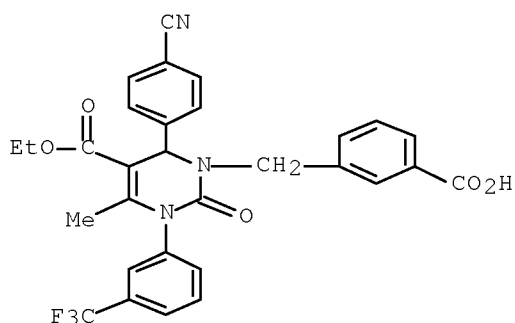
RN 904958-60-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[[3-(methoxycarbonyl)phenyl]methyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-61-8 ZCAPLUS

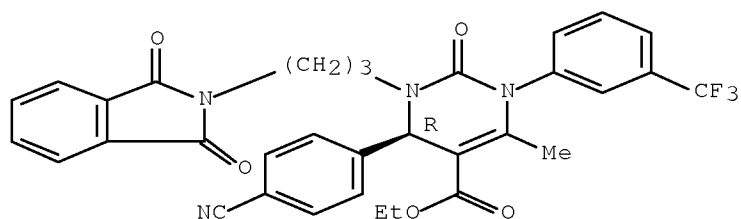
CN 5-Pyrimidinecarboxylic acid, 3-[(3-carboxyphenyl)methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 5-ethyl ester (CA INDEX NAME)



RN 904958-62-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

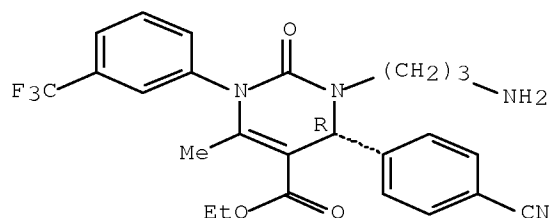
Absolute stereochemistry.



RN 904958-63-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(3-aminopropyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

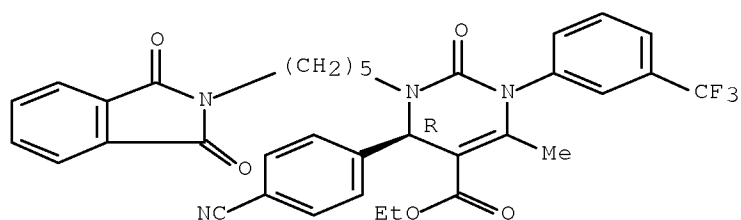
Absolute stereochemistry.



RN 904958-64-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[5-(1,3-dihydro-1,3-dioxo-2H-isindol-2-yl)pentyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

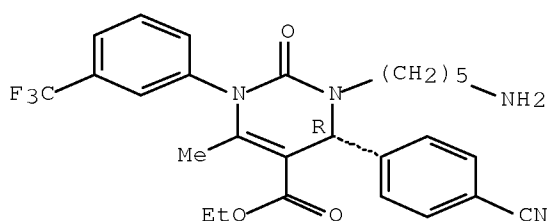
Absolute stereochemistry.



RN 904958-65-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(5-aminopentyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

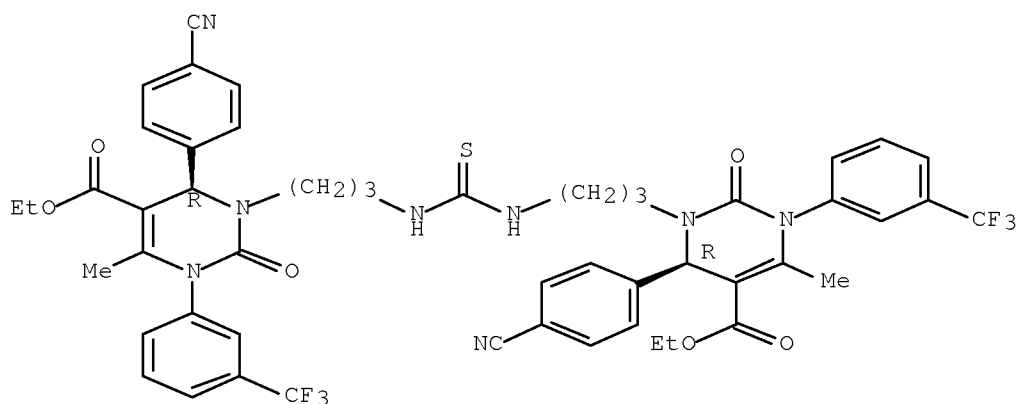
Absolute stereochemistry.



RN 904958-66-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[carbonothioylbis(imino-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

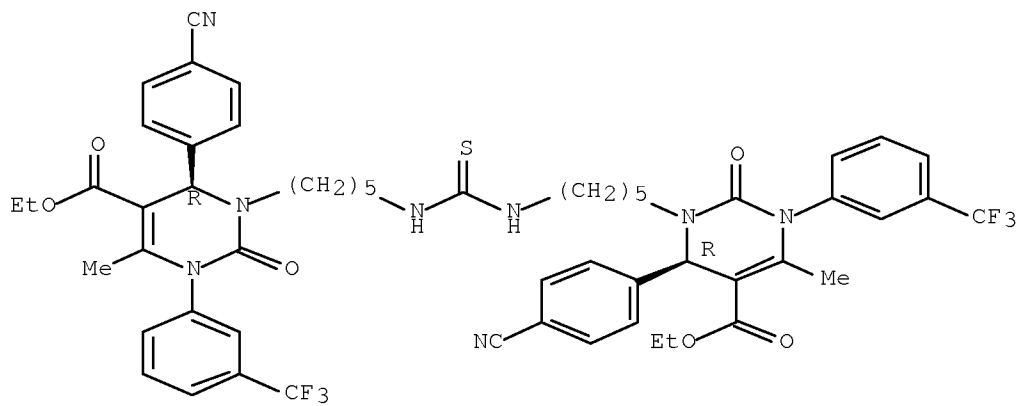
Absolute stereochemistry.



RN 904958-67-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[carbonothioylbis(imino-5,1-pentanediy)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

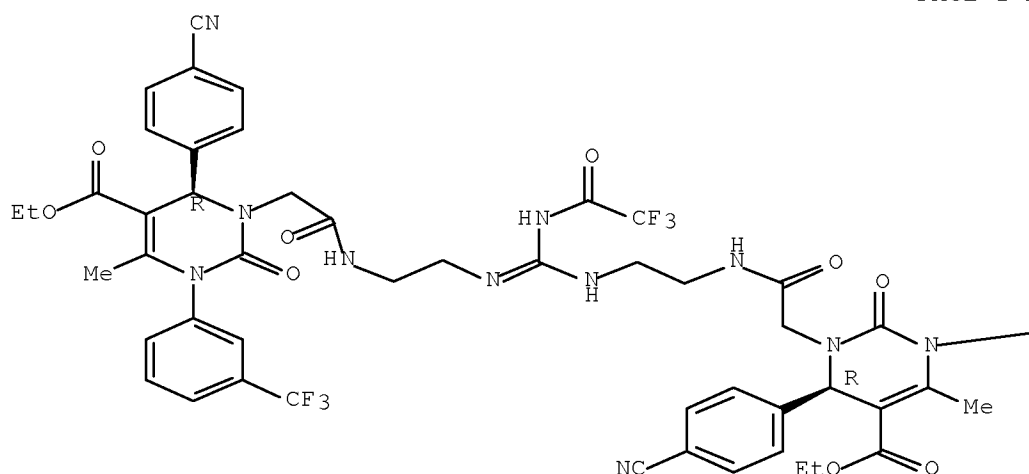


RN 904958-68-5 ZCAPLUS

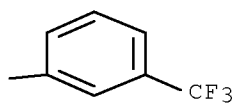
CN 5-Pyrimidinecarboxylic acid, 1,1'-[2,12-dioxo-7-[(trifluoroacetyl)amino]-3,6,8,11-tetraaza-6-tridecene-1,13-diyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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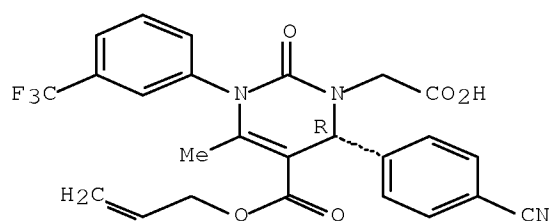
PAGE 1-B



RN 904958-69-6 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.

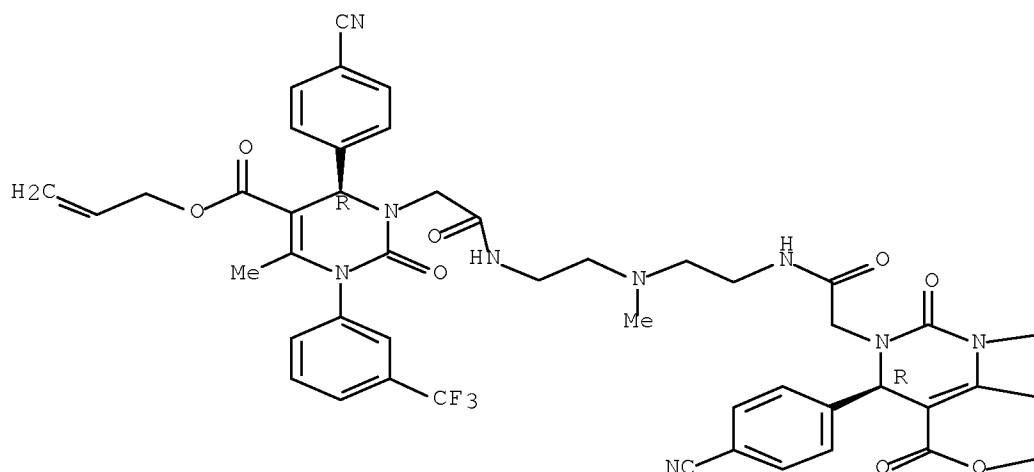


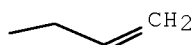
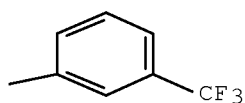
RN 904958-70-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-[[2-[[2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

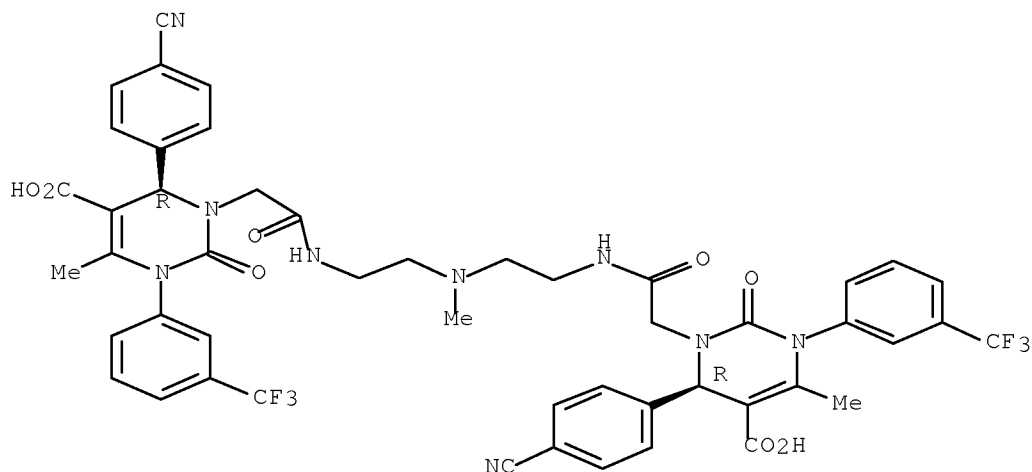




RN 904958-71-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[2-[[2-[[2-[[2-[(6R)-5-carboxy-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R)- (CA INDEX NAME)

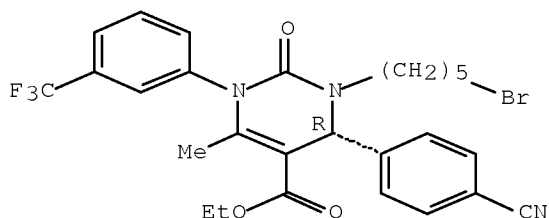
Absolute stereochemistry.



RN 904958-72-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(5-bromopentyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

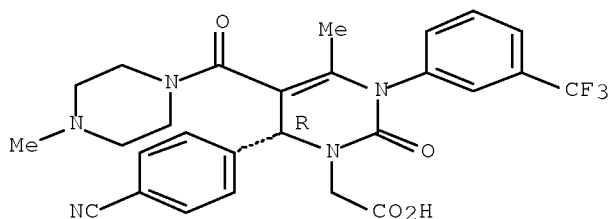
Absolute stereochemistry.



RN 904958-75-4 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-[(4-methyl-1-piperazinyl)carbonyl]-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

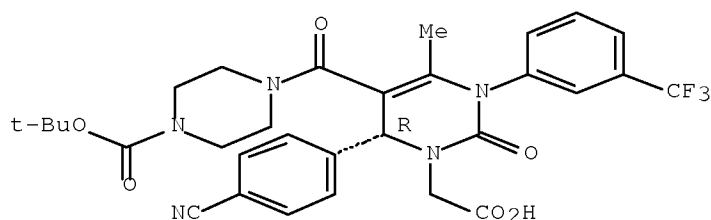
Absolute stereochemistry.



RN 904958-76-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-[[4-[(1,1-dimethylethoxy)carbonyl]-1-piperazinyl]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.

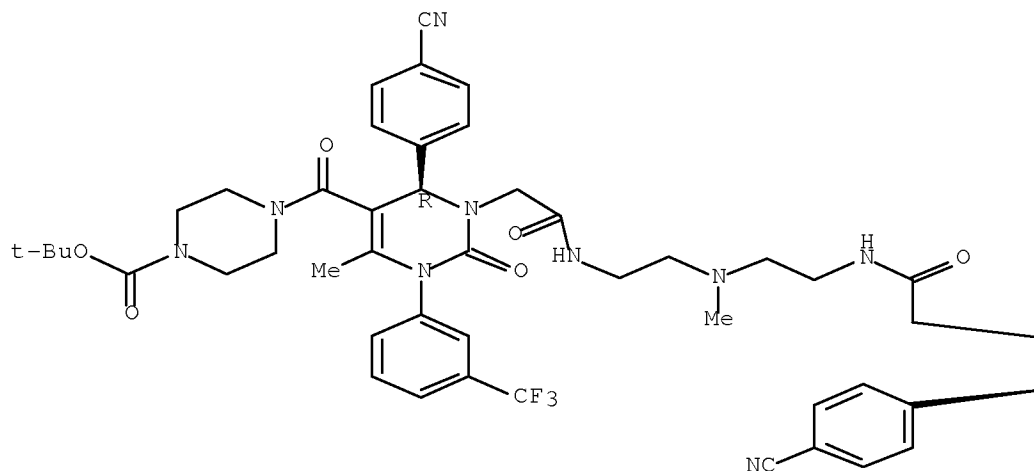


RN 904958-77-6 ZCAPLUS

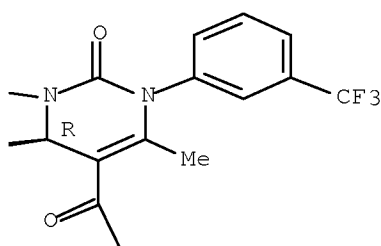
CN 1-Piperazinecarboxylic acid, 4-[[[(4R)-4-(4-cyanophenyl)-3-[2-[[2-[[2-[[2-[(6R)-6-(4-cyanophenyl)-5-[[4-[(1,1-dimethylethoxy)carbonyl]-1-piperazinyl]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.

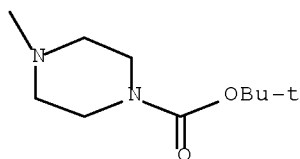
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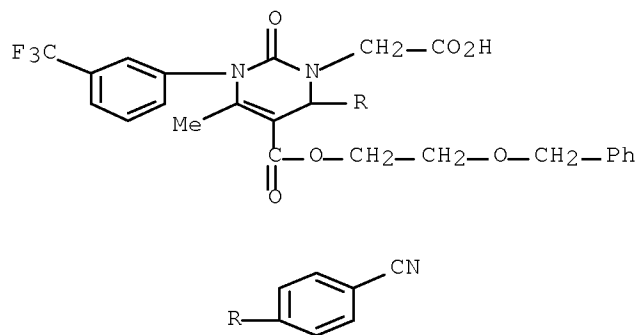
PAGE 1-B



PAGE 2-B



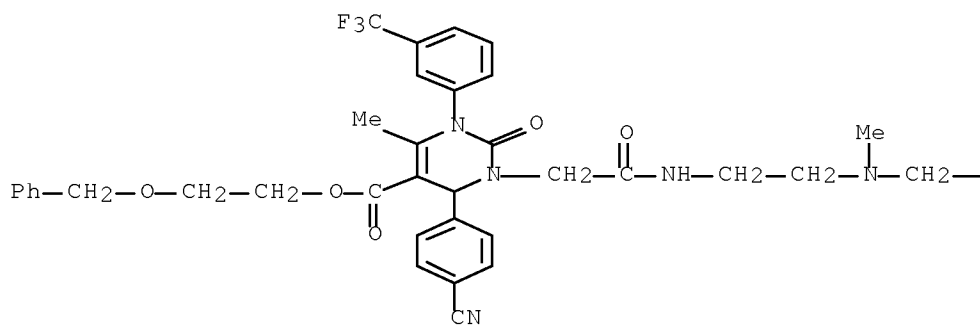
RN 904958-79-8 ZCAPLUS
 CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[2-(phenylmethoxy)ethoxy]carbonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



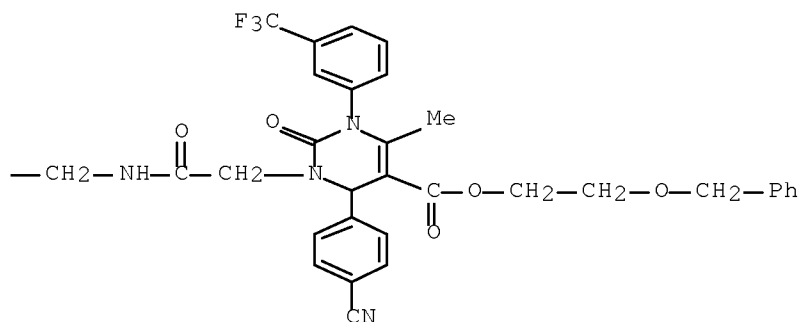
RN 904958-80-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-[[2-[[2-[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[2-(phenylmethoxy)ethoxy]carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(phenylmethoxy)ethyl ester (CA INDEX NAME)

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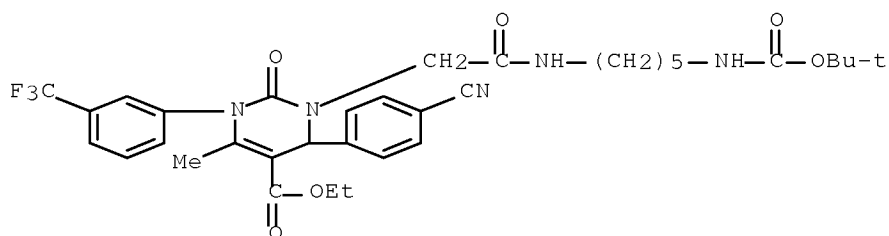


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RN 904958-81-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[5-[[[(1,1-dimethylethoxy)carbonyl]amino]pentyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



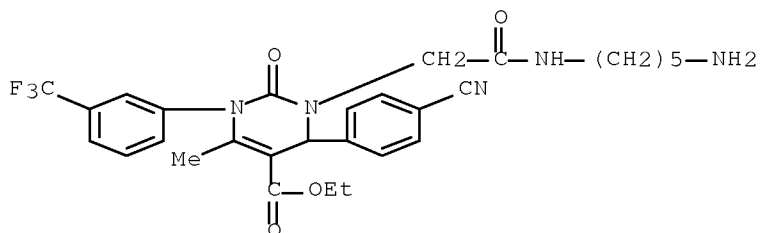
RN 904958-83-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[2-[(5-aminopentyl)amino]-2-oxoethyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 904958-82-3

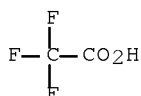
CMF C29 H32 F3 N5 O4



CM 2

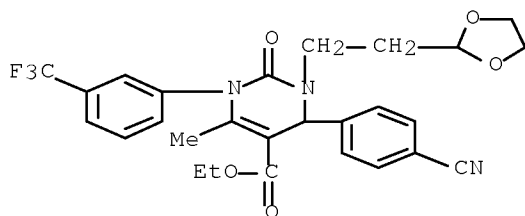
CRN 76-05-1

CMF C2 H F3 O2



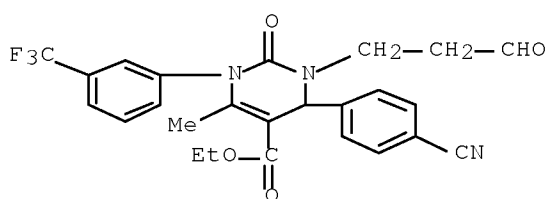
RN 904958-97-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-(1,3-dioxolan-2-yl)ethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-98-1 ZCAPLUS

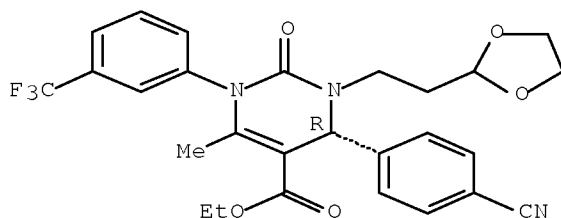
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(3-oxopropyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-99-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-(1,3-dioxolan-2-yl)ethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

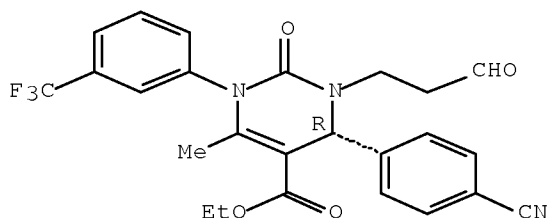
Absolute stereochemistry.



RN 904959-00-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(3-oxopropyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

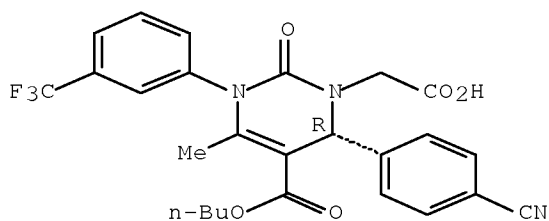
Absolute stereochemistry.



RN 904959-03-1 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-(butoxycarbonyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

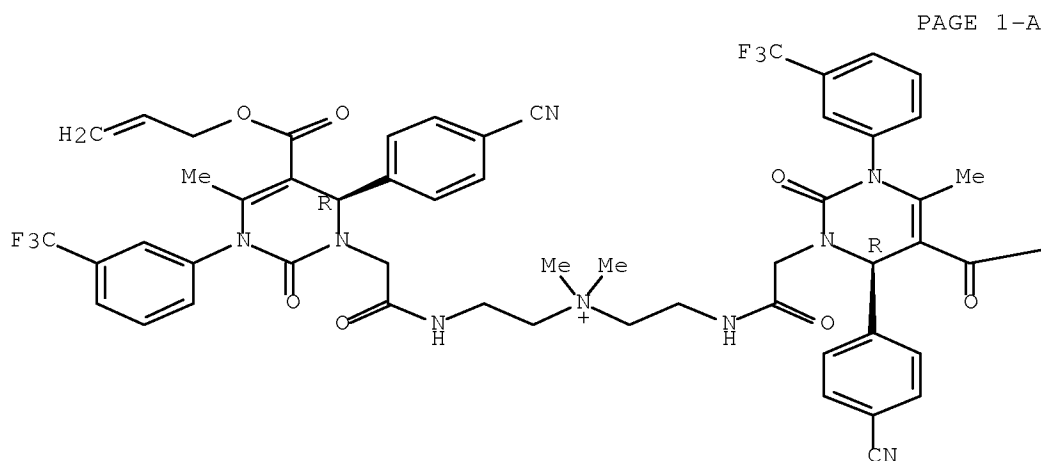
Absolute stereochemistry.



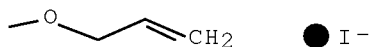
RN 904959-04-2 ZCAPLUS

CN Ethanaminium, 2-[[2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.



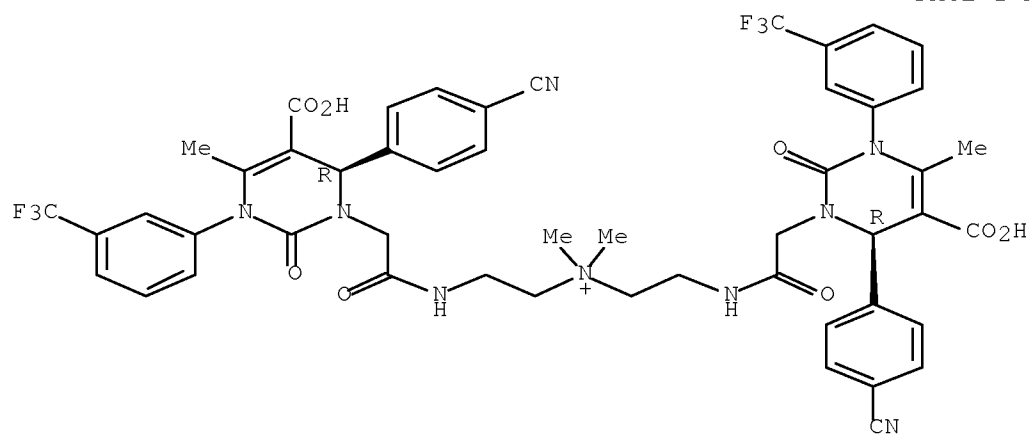
PAGE 1-B



RN 904959-05-3 ZCAPLUS
 CN Ethanaminium, 2-[[2-[(6R)-5-carboxy-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[(6R)-5-carboxy-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

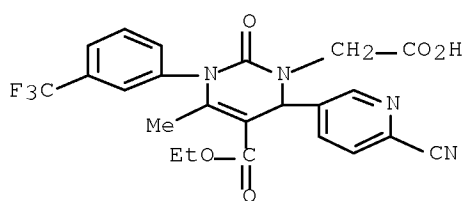
PAGE 1-A



PAGE 2-A



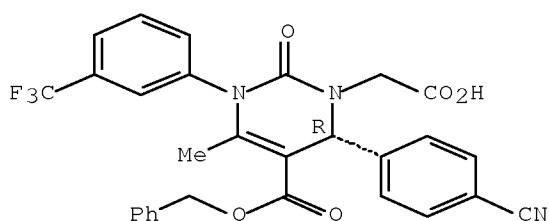
RN 904959-06-4 ZCAPLUS
 CN 1(2H)-Pyrimidineacetic acid, 6-(6-cyano-3-pyridinyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 904959-08-6 ZCAPLUS

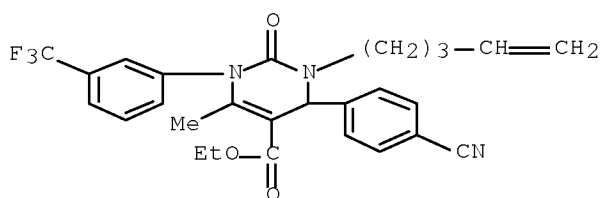
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(phenylmethoxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 904959-16-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(4-penten-1-yl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



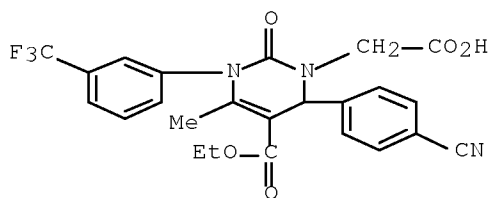
IT 671776-27-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of multimers of tetrahydropyrimidinone compds. as elastase inhibitors useful in the treatment of respiratory diseases)

RN 671776-27-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L6 ANSWER 5 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:979623 ZCAPLUS Full-text
 DOCUMENT NUMBER: 143:286441
 TITLE: Preparation of diaryl-dihydropyrimidin-2-ones as human neutrophil elastase inhibitors
 INVENTOR(S): Gielen-Haertwig, Heike; Albrecht, Barbara; Keldenich, Joerg; Li, Volkhart; Pernerstorfer, Josef; Schlemmer, Karl-Heinz; Telan, Leila
 PATENT ASSIGNEE(S): Bayer Healthcare A.-G., Germany
 SOURCE: PCT Int. Appl., 141 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|-----------------|------------|
| WO 2005082864 | A1 | 20050909 | WO 2005-EP1486 | 20050215 |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | |
| RW: | BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
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| EP 1723121 | A1 | 20061122 | EP 2005-707386 | 20050215 |
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| JP 2007524696 | T | 20070830 | JP 2007-500099 | 20050215 |
| US 20080064704 | A1 | 20080313 | US 2007-590770 | 20070618 |
| PRIORITY APPLN. INFO.: | | | EP 2004-4314 | A 20040226 |
| | | | WO 2005-EP1486 | W 20050215 |
| OTHER SOURCE(S): | CASREACT 143:286441; MARPAT 143:286441 | | | |
| GI | | | | |

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [A = aryl or heteroaryl ring; R1, R2 and R3 independently = H, halo, nitro, etc.; R4 = (un)substituted alkyl, cycloalkylcarbonyl,

alkylcarbonyl, etc.; R5 = (un)substituted alkyl; R6 = H, formyl, aminocarbonyl, etc.; R7 = cyano, OH, nitro, etc.; V, W, X, Y and Z independently = CH or N wherein the ring contains either 0, 1 or 2 nitrogen atoms] and their pharmaceutically acceptable salts, are prepared and disclosed as human neutrophil elastase (HNE) inhibitors. Thus, e.g., II was prepared by cyclization of N-[3-(trifluoromethyl)phenyl]urea and 4-cyanobenzaldehyde with ethyl-3-oxobutanoate and subsequent reduction using LAH. The activity of I against HNE was evaluated in an in vitro enzyme assay utilizing a fluorogenic peptide substrate and it was revealed that selected compds. of the invention possessed IC₅₀ values in the range of 5 up to 1000 nM. I as inhibitors of human neutrophil elastase should prove useful in the treatment of chronic obstructive pulmonary diseases, acute coronary syndrome, acute myocardial infarction and heart failure development. Pharmaceutical compns. comprising I are disclosed.

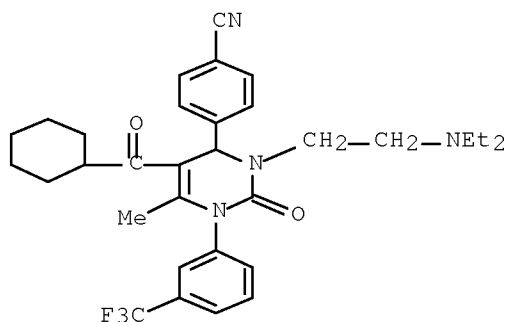
IT 864251-32-1P 864251-33-2P

RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(preparation of diaryl-dihydropyrimidin-2-ones as human neutrophil elastase inhibitors)

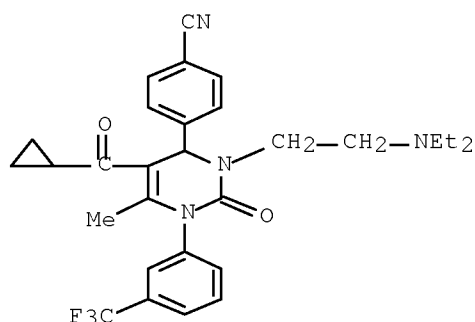
RN 864251-32-1 ZCAPLUS

CN Benzonitrile, 4-[5-(cyclohexylcarbonyl)-3-[2-(diethylamino)ethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]-(CA INDEX NAME)



RN 864251-33-2 ZCAPLUS

CN Benzonitrile, 4-[5-(cyclopropylcarbonyl)-3-[2-(diethylamino)ethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]-(CA INDEX NAME)



IT 864251-36-5P 864251-37-6P

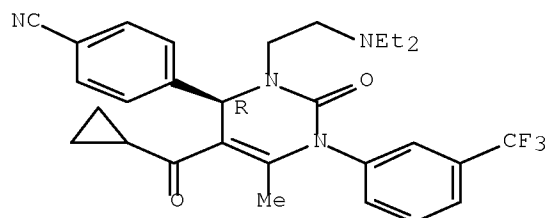
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of diaryl-dihydropyrimidin-2-ones as human neutrophil elastase inhibitors)

RN 864251-36-5 ZCAPLUS

CN Benzonitrile, 4-[(4R)-5-(cyclopropylcarbonyl)-3-[2-(diethylamino)ethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]- (CA INDEX NAME)

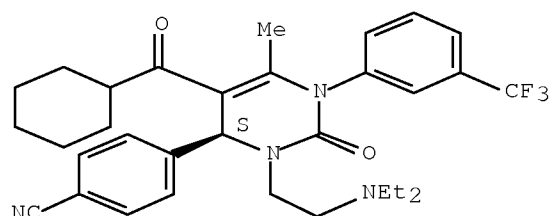
Absolute stereochemistry.



RN 864251-37-6 ZCAPLUS

CN Benzonitrile, 4-[(4S)-5-(cyclohexylcarbonyl)-3-[2-(diethylamino)ethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]- (CA INDEX NAME)

Absolute stereochemistry.



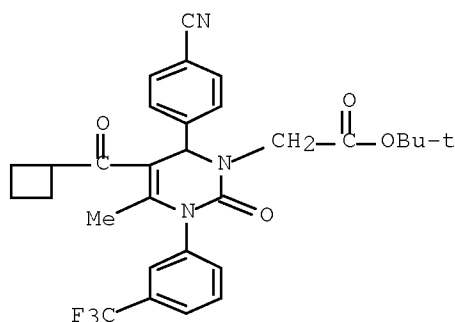
IT 864250-66-8P 864250-67-9P 864250-68-0P
864250-71-5P 864250-72-6P 864250-73-7P
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864250-83-9P 864250-86-2P 864250-87-3P
 864250-95-3P 864251-05-8P 864251-08-1P
 864251-09-2P 864251-10-5P 864251-22-9P
 864251-24-1P 864251-27-4P 864251-29-6P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (preparation of diaryl-dihydropyrimidin-2-ones as human neutrophil elastase inhibitors)

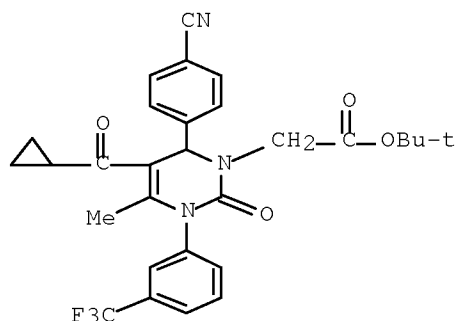
RN 864250-66-8 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclobutylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



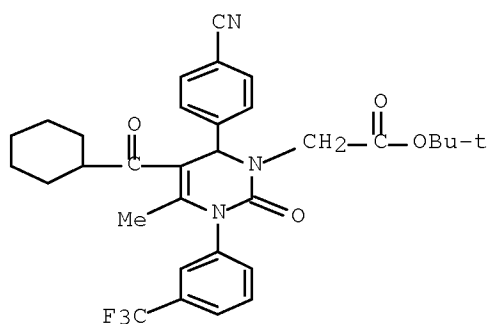
RN 864250-67-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



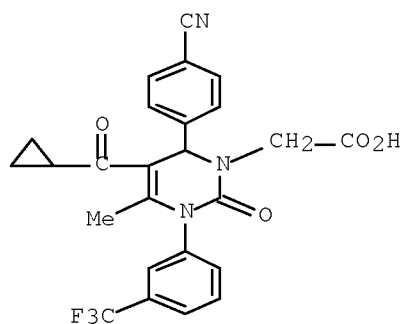
RN 864250-68-0 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



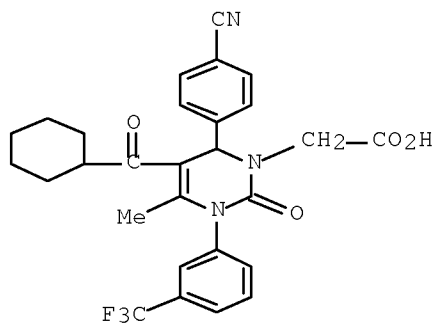
RN 864250-71-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



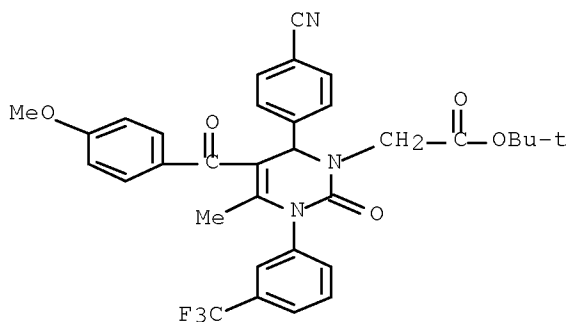
RN 864250-72-6 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



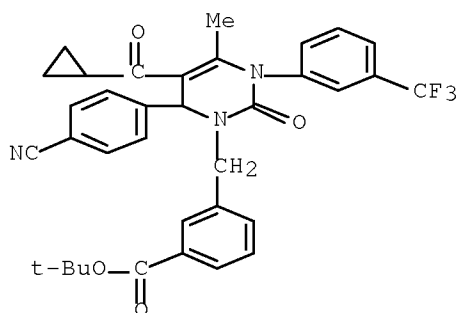
RN 864250-73-7 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-5-(4-methoxybenzoyl)-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



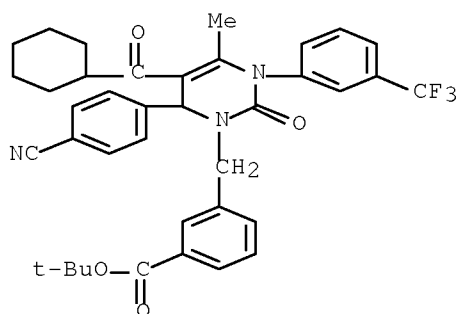
RN 864250-75-9 ZCAPLUS

CN Benzoic acid, 3-[[6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



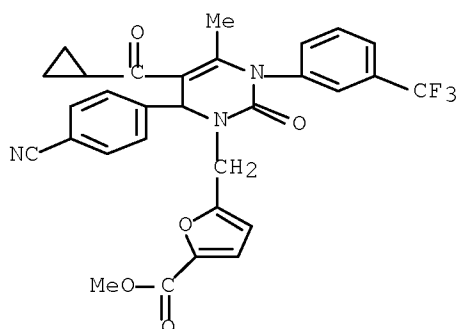
RN 864250-78-2 ZCAPLUS

CN Benzoic acid, 3-[[6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



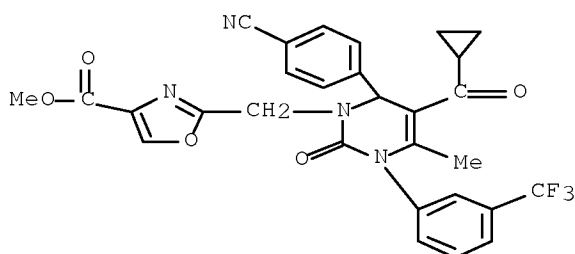
RN 864250-82-8 ZCAPLUS

CN 2-Furancarboxylic acid, 5-[[6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



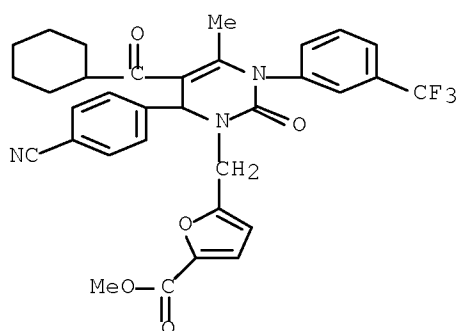
RN 864250-83-9 ZCAPLUS

CN 4-Oxazolecaboxylic acid, 2-[[6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



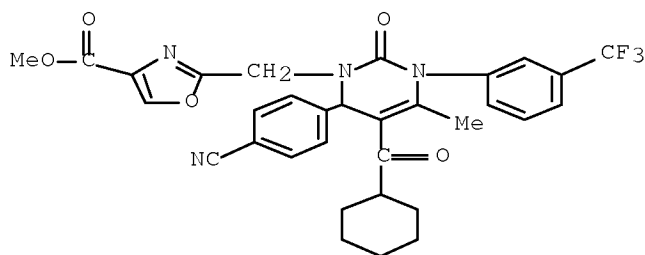
RN 864250-86-2 ZCAPLUS

CN 2-Furancarboxylic acid, 5-[[6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



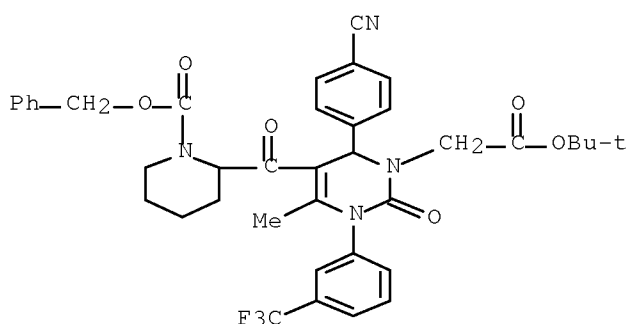
RN 864250-87-3 ZCAPLUS

CN 4-Oxazolecaboxylic acid, 2-[[6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



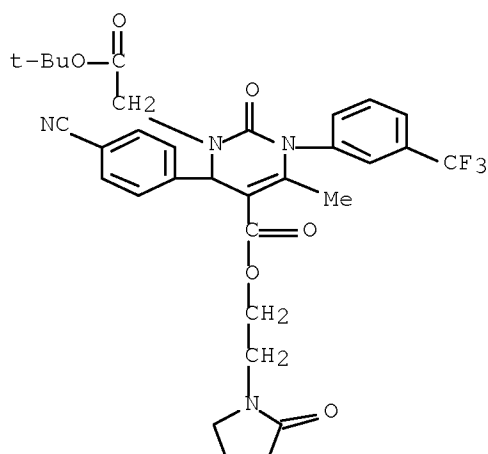
RN 864250-95-3 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[1-[(phenylmethoxy)carbonyl]-2-piperidinyl]carbonyl]-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864251-05-8 ZCAPLUS

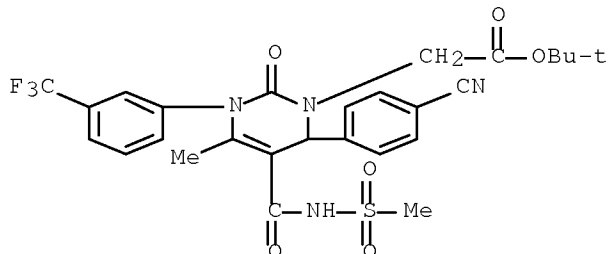
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[2-(2-oxo-1-pyrrolidinyl)ethoxy]carbonyl]-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864251-08-1 ZCAPLUS

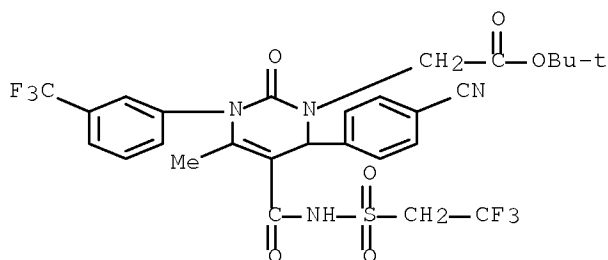
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-[[(methylsulfonyl) amino]carbonyl]-2-oxo-3-[3-(trifluoromethyl)phenyl]-,

1,1-dimethylethyl ester (CA INDEX NAME)



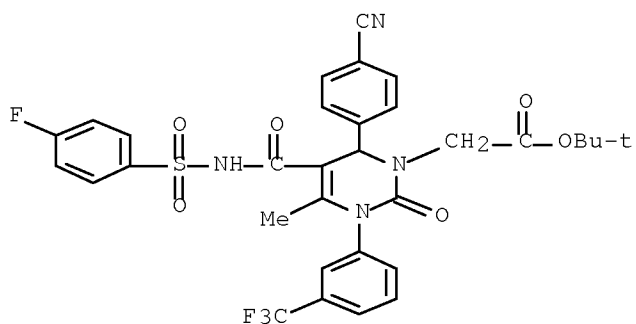
RN 864251-09-2 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[[(2,2,2-trifluoroethyl)sulfonyl]amino]carbonyl]-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



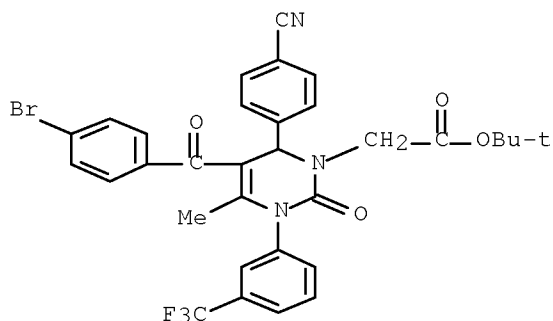
RN 864251-10-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-[[[(4-fluorophenyl)sulfonyl]amino]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



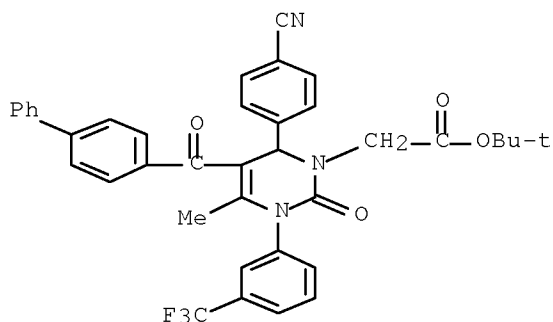
RN 864251-22-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-(4-bromobenzoyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



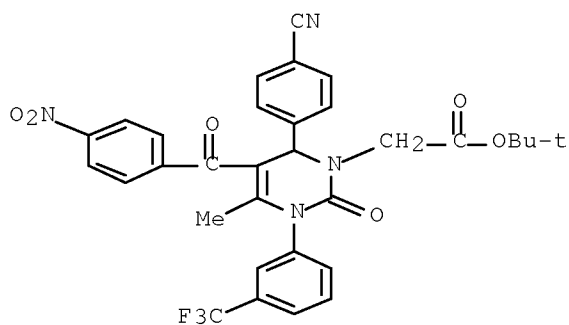
RN 864251-24-1 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-([1,1'-biphenyl]-4-ylcarbonyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864251-27-4 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(4-nitrobenzoyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

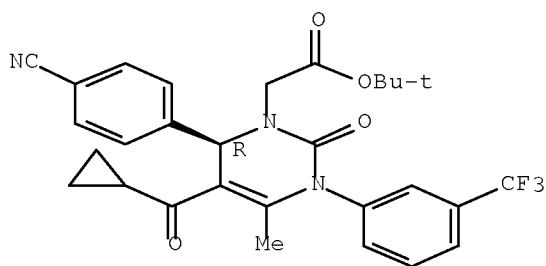


RN 864251-29-6 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

ester, (6R)- (CA INDEX NAME)

Absolute stereochemistry.



IT 864250-45-3P 864250-69-1P 864250-70-4P
 864250-74-8P 864250-76-0P 864250-79-3P
 864250-80-6P 864250-84-0P 864250-85-1P
 864250-88-4P 864250-89-5P 864250-90-8P
 864250-91-9P 864250-92-0P 864250-93-1P
 864250-96-4P 864251-02-5P 864251-03-6P
 864251-04-7P 864251-06-9P 864251-07-0P
 864251-14-9P 864251-15-0P 864251-16-1P
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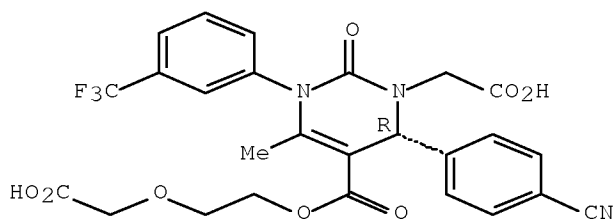
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of diaryl-dihydropyrimidin-2-ones as human neutrophil elastase inhibitors)

RN 864250-45-3 ZCAPLUS

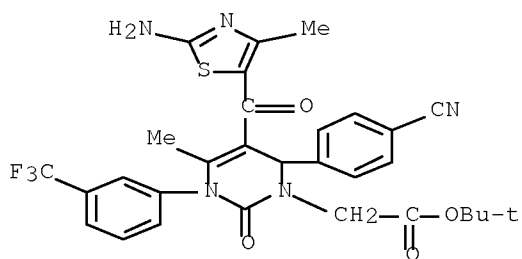
CN 1(2H)-Pyrimidineacetic acid, 5-[[2-(carboxymethoxy)ethoxy]carbonyl]-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.



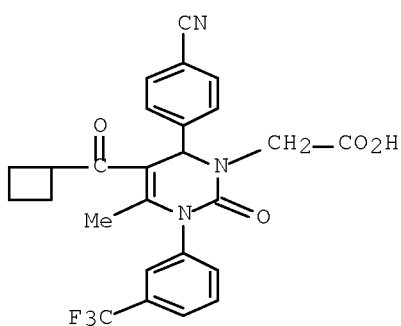
RN 864250-69-1 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-[(2-amino-4-methyl-5-thiazolyl)carbonyl]-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



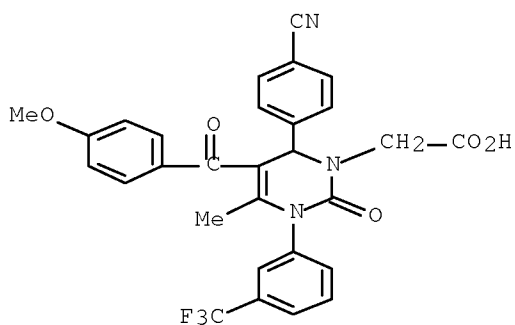
RN 864250-70-4 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclobutylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



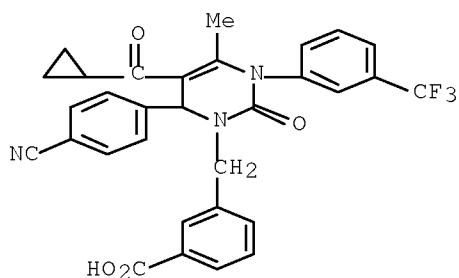
RN 864250-74-8 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-5-(4-methoxybenzoyl)-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



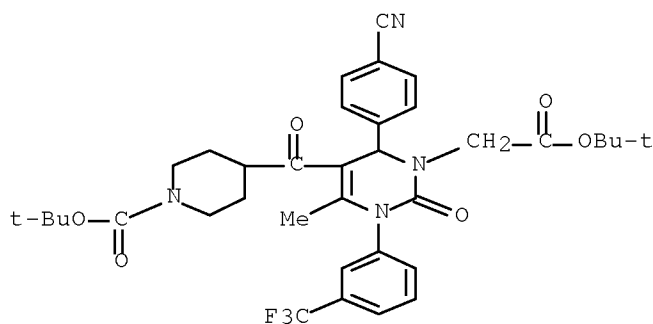
RN 864250-76-0 ZCAPLUS

CN Benzoic acid, 3-[[6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



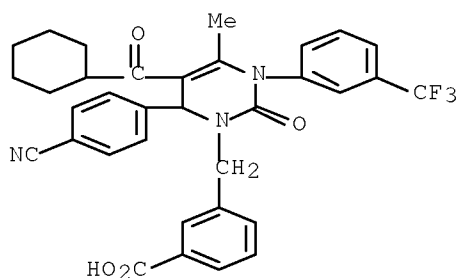
RN 864250-79-3 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-[[1-[(1,1-dimethylethoxy)carbonyl]-4-piperidinyl]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



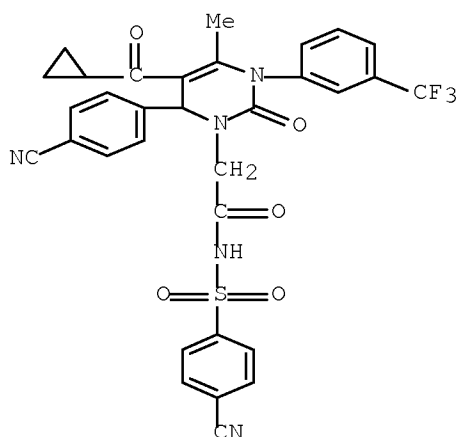
RN 864250-80-6 ZCAPLUS

CN Benzoic acid, 3-[[6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



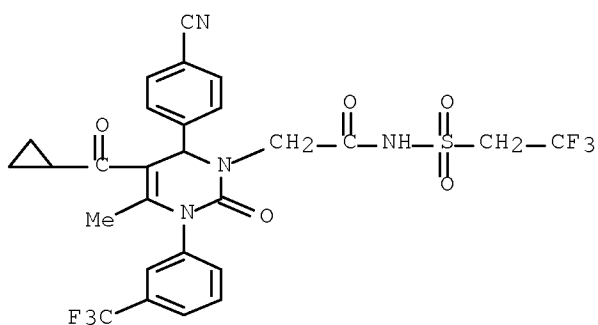
RN 864250-84-0 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-N-[(4-cyanophenyl)sulfonyl]-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



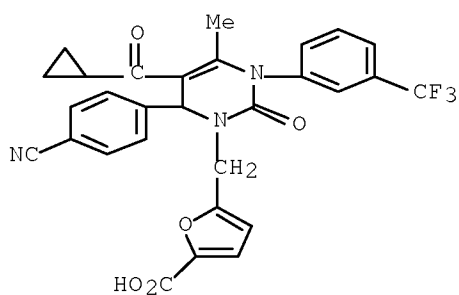
RN 864250-85-1 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-N-[(2,2,2-trifluoroethyl)sulfonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864250-88-4 ZCAPLUS

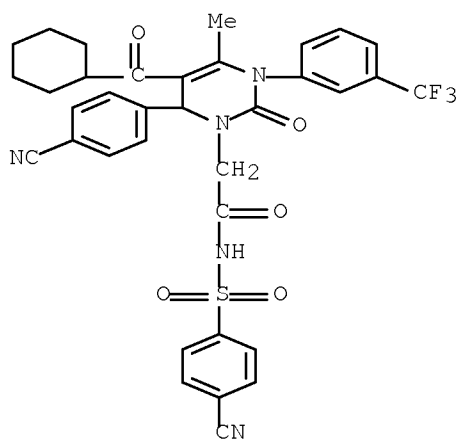
CN 2-Furancarboxylic acid, 5-[[6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



RN 864250-89-5 ZCAPLUS

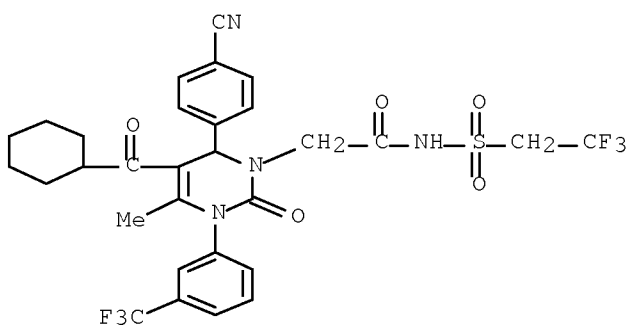
CN 1(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-N-[(4-cyanophenyl)sulfonyl]-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



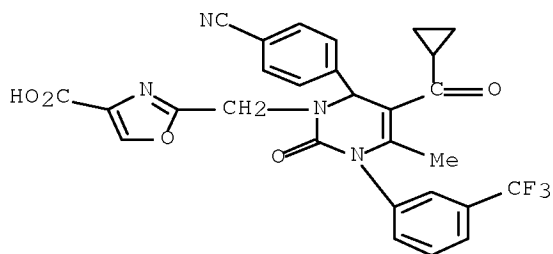
RN 864250-90-8 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-N-[(2,2,2-trifluoroethyl)sulfonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

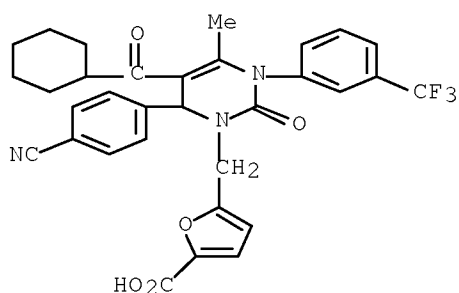


RN 864250-91-9 ZCAPLUS

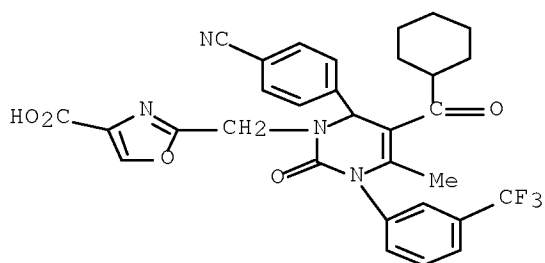
CN 4-Oxazolecarboxylic acid, 2-[[6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



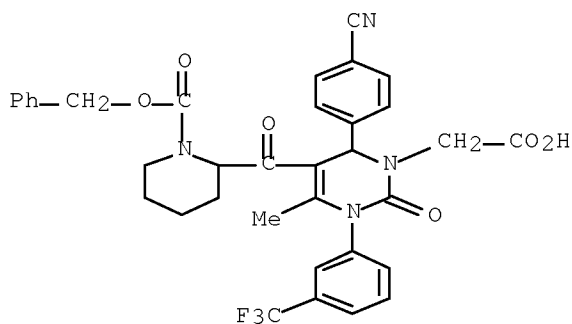
RN 864250-92-0 ZCAPLUS
 CN 2-Furancarboxylic acid, 5-[[6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



RN 864250-93-1 ZCAPLUS
 CN 4-Oxazolecarboxylic acid, 2-[[6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)

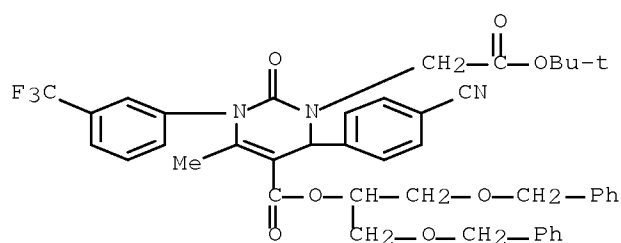


RN 864250-96-4 ZCAPLUS
 CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[1-[(phenylmethoxy)carbonyl]-2-piperidinyl]carbonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864251-02-5 ZCAPLUS

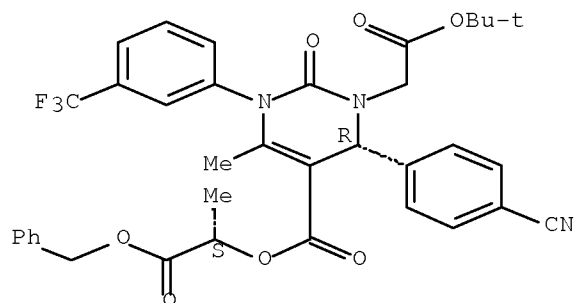
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[2-(phenylmethoxy)-1-[(phenylmethoxy)methyl]ethoxy]carbonyl]-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864251-03-6 ZCAPLUS

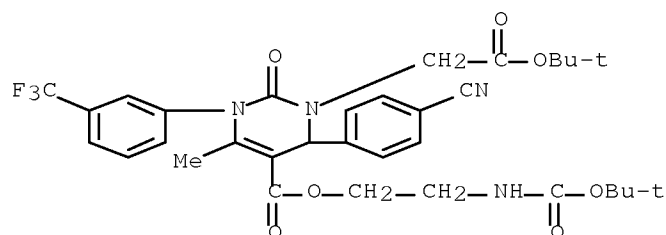
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-[[[(1S)-1-methyl-2-oxo-2-(phenylmethoxy)ethoxy]carbonyl]-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, (6R)-rel- (CA INDEX NAME)

Relative stereochemistry.



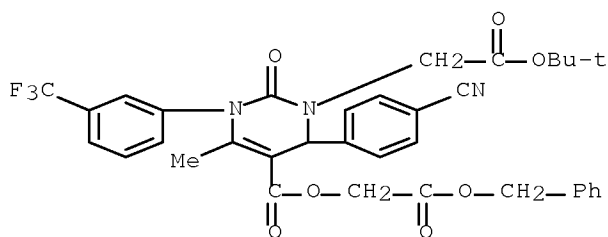
RN 864251-04-7 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-[[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethoxy]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



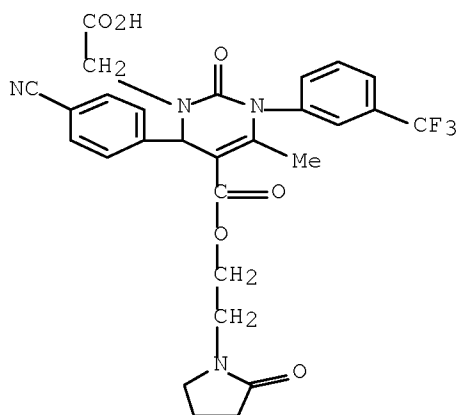
RN 864251-06-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[2-oxo-2-(phenylmethoxy)ethoxy]carbonyl]-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



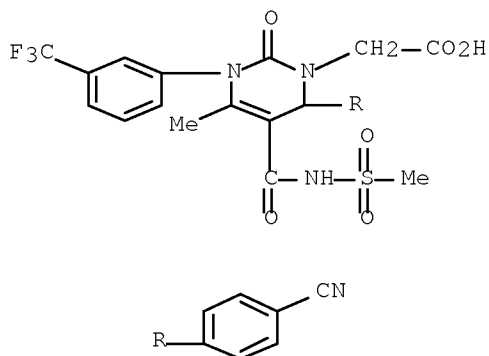
RN 864251-07-0 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[2-(2-oxo-1-pyrrolidinyl)ethoxy]carbonyl]-3-[3-(trifluoromethyl)phenyl]-
(CA INDEX NAME)



RN 864251-14-9 ZCAPLUS

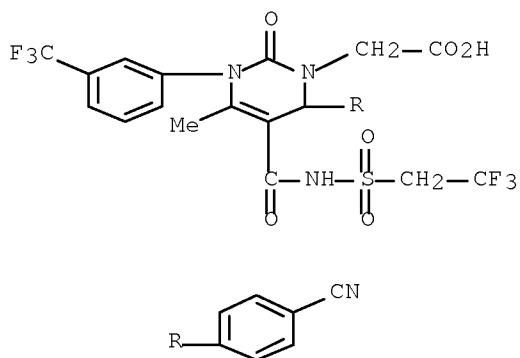
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-[[(methylsulfonyl) amino]carbonyl]-2-oxo-3-[3-(trifluoromethyl)phenyl]-
(CA INDEX NAME)



RN 864251-15-0 ZCAPLUS

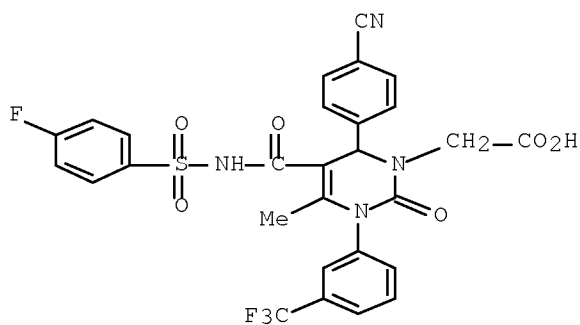
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-

5-[[[(2,2,2-trifluoroethyl)sulfonyl]amino]carbonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



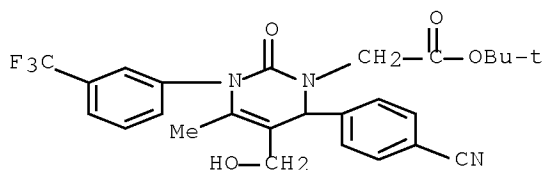
RN 864251-16-1 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-[[[(4-fluorophenyl)sulfonyl]amino]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



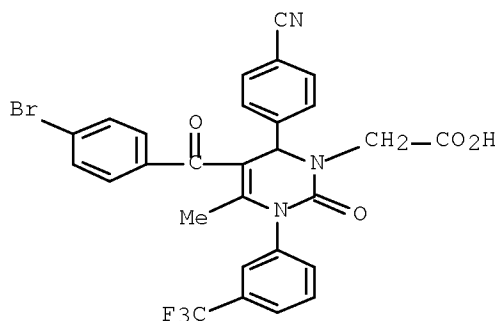
RN 864251-17-2 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-5-(hydroxymethyl)-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



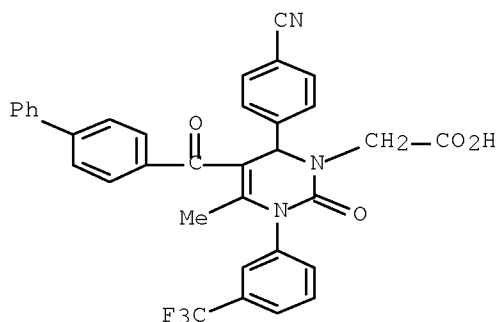
RN 864251-23-0 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-(4-bromobenzoyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



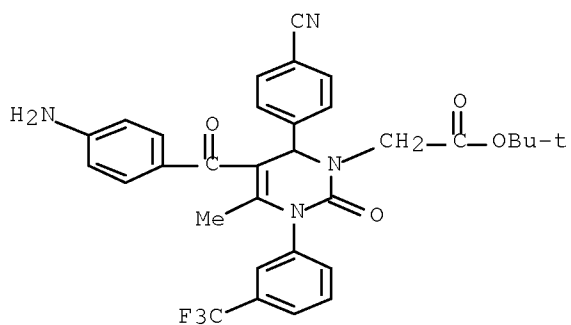
RN 864251-25-2 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-([1,1'-biphenyl]-4-ylcarbonyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864251-28-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-(4-aminobenzoyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

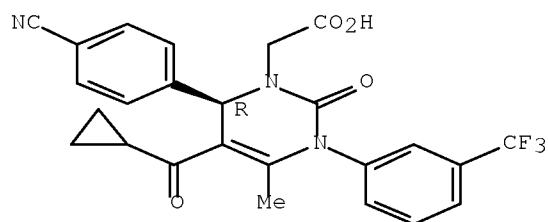


RN 864251-30-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

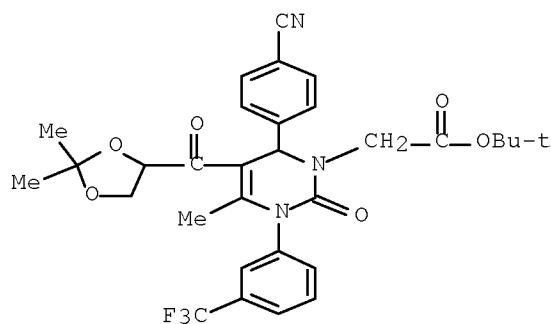
NAME)

Absolute stereochemistry.



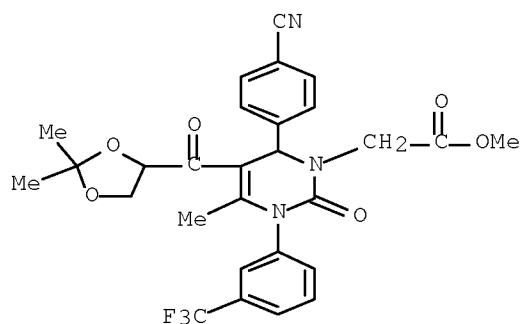
RN 864251-34-3 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-[(2,2-dimethyl-1,3-dioxolan-4-yl)carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864251-35-4 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-[(2,2-dimethyl-1,3-dioxolan-4-yl)carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, methyl ester (CA INDEX NAME)



IT 864151-39-3P 864251-40-1P 864251-41-2F

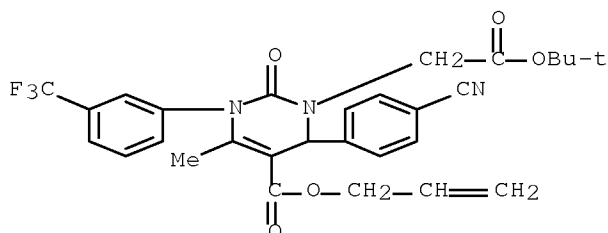
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of diaryl-dihydropyrimidin-2-ones as human neutrophil elastase

inhibitors)

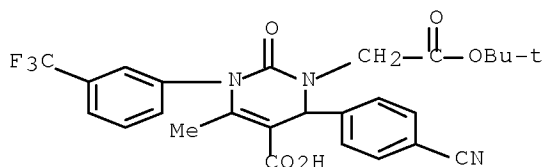
RN 864151-39-3 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



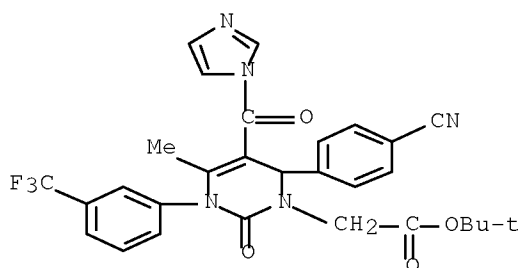
RN 864251-40-1 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-carboxy-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1-(1,1-dimethylethyl) ester (CA INDEX NAME)



RN 864251-41-2 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-5-(1H-imidazol-1-ylcarbonyl)-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:979622 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:286440

TITLE: Preparation of tetrasubstituted pyrimidin-2-ones as

human neutrophil elastase inhibitors

INVENTOR(S): Gielen-Haertwig, Heike; Albrecht, Barbara; Keldenich, Joerg; Li, Volkhart; Pernerstorfer, Josef; Schlemmer, Karl-Heinz; Telan, Leila

PATENT ASSIGNEE(S): Bayer Healthcare A.-G., Germany

SOURCE: PCT Int. Appl., 119 pp.
CODEN: PIXXD2

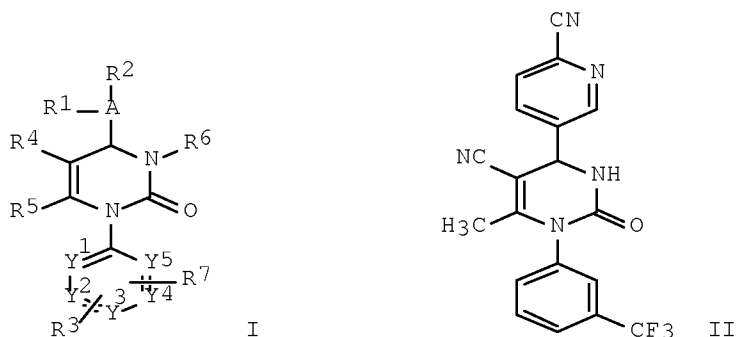
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|----------|-------------------|------------|
| WO 2005082863 | A2 | 20050909 | WO 2005-EP1487 | 20050215 |
| WO 2005082863 | A3 | 20051222 | | |
| <p>W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW</p> <p>RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG</p> | | | | |
| CA 2557272 | A1 | 20050909 | CA 2005-2557272 | 20050215 |
| EP 1730121 | A2 | 20061213 | EP 2005-707387 | 20050215 |
| <p>R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR</p> | | | | |
| JP 2007523931 | T | 20070823 | JP 2007-500100 | 20050215 |
| US 20080021053 | A1 | 20080124 | US 2007-590786 | 20070720 |
| PRIORITY APPLN. INFO.: | | | EP 2004-4315 | A 20040226 |
| | | | WO 2005-EP1487 | W 20050215 |
| OTHER SOURCE(S): | | | MARPAT 143:286440 | |
| GI | | | | |



AB Title compds. I [A = heteroaryl ring; R1-3 = H, halo, NO₂, etc.; R4 = CF₃CO, alkylcarbonyl, etc.; R5 = alkyl, alkoxy, etc.; R6 = T-U; T = alkanediyl, akenediyl; U = aryl, heteroaryl, etc.; R7 = halo, NO₂, CN, etc.; Y1-5 = independently CH, N wherein the ring contains 0-2 N atoms] and analogs are prepared For instance, II is prepared in 6 steps from 2-bromo-5-

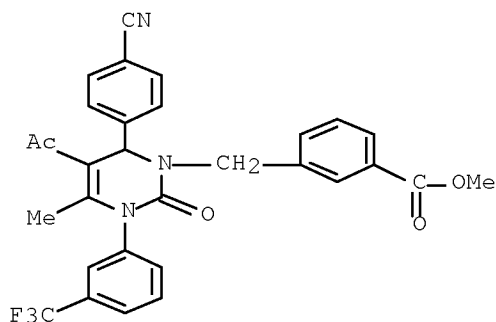
methylpyridine, allyl 3-oxobutanoate and N-[3- (trifluoromethyl)phenyl]urea. II has an IC₅₀ = 70 nM for human neutrophil elastase (HNE). I are useful for the treatment of chronic obstructive pulmonary diseases, acute coronary syndrome, acute myocardial infarction and heart failure development.

IT 864150-42-5P 864150-44-7P 864150-46-9P
 864150-48-1P 864150-50-5P 864150-52-7P
 864150-53-8P 864150-54-9P 864150-55-0P
 864150-56-1P 864150-57-2P 864150-58-3P
 864150-59-4P 864150-60-7P 864150-61-8P
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 864150-81-2P 864150-82-3P 864150-83-4P
 864150-86-7P 864150-89-0P 864150-93-6P
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 864151-12-2P 864151-29-1P 864151-50-8P
 864151-51-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (preparation of tetrasubstituted pyrimidin-2-ones as human neutrophil elastase inhibitors)

RN 864150-42-5 ZCAPLUS

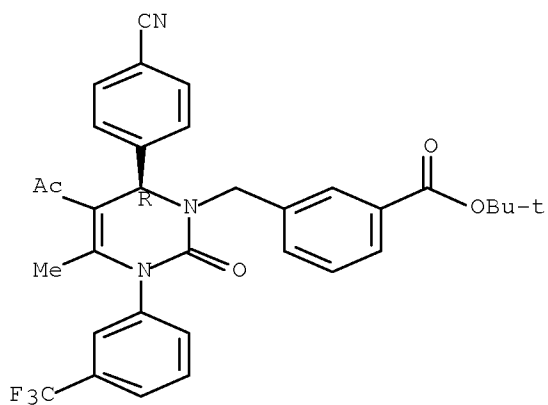
CN Benzoic acid, 3-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



RN 864150-44-7 ZCAPLUS

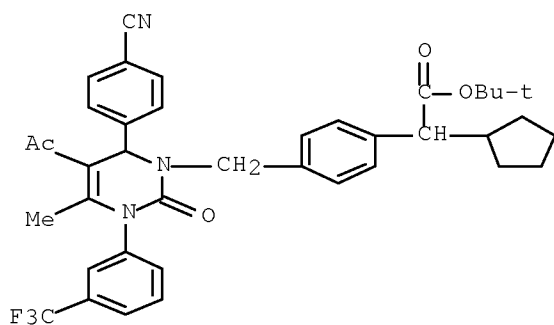
CN Benzoic acid, 3-[[[(6R)-5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



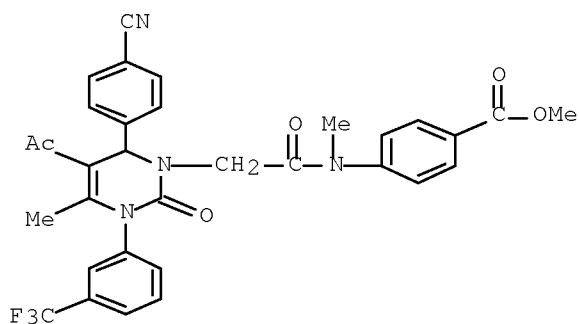
RN 864150-46-9 ZCAPLUS

CN Benzeneacetic acid, 4-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-α-cyclopentyl-, 1,1-dimethylethyl ester (CA INDEX NAME)



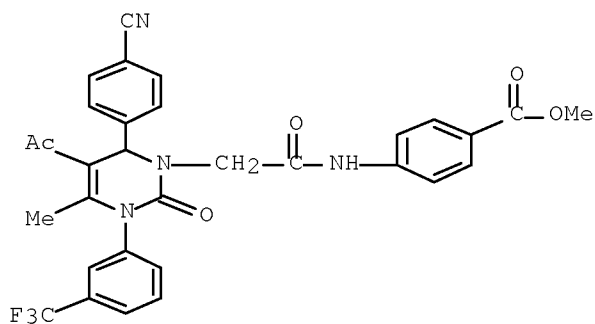
RN 864150-48-1 ZCAPLUS

CN Benzoic acid, 4-[[2-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]methylamino]-, methyl ester (CA INDEX NAME)



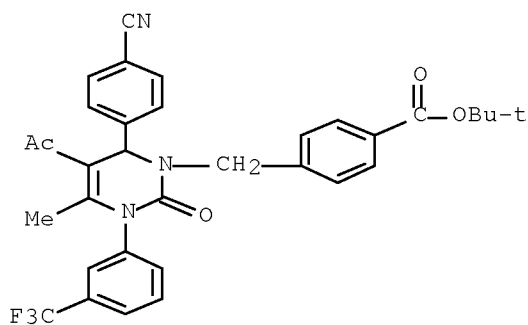
RN 864150-50-5 ZCAPLUS

CN Benzoic acid, 4-[[2-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-, methyl ester (CA INDEX NAME)



RN 864150-52-7 ZCAPLUS

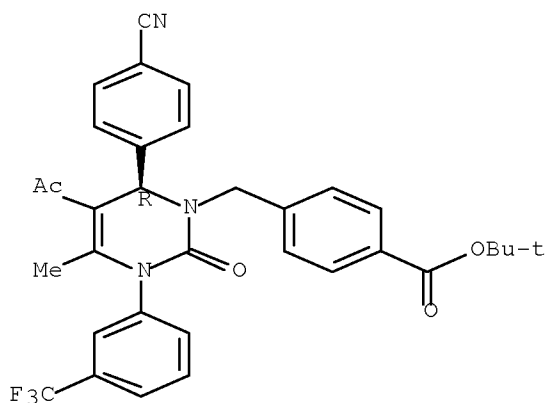
CN Benzoic acid, 4-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864150-53-8 ZCAPLUS

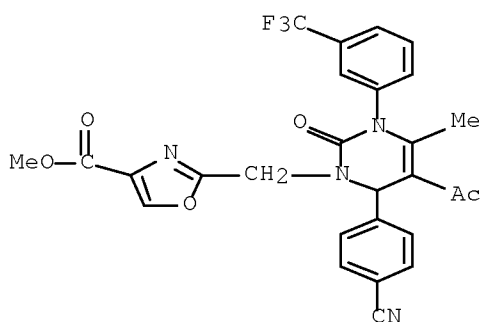
CN Benzoic acid, 4-[[[(6R)-5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 864150-54-9 ZCAPLUS

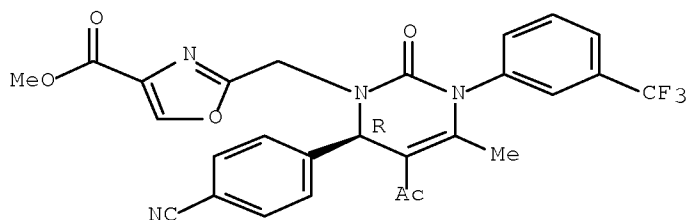
CN 4-Oxazolecaboxylic acid, 2-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



RN 864150-55-0 ZCAPLUS

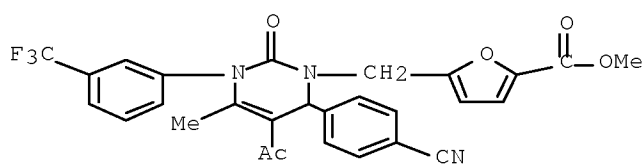
CN 4-Oxazolecaboxylic acid, 2-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 864150-56-1 ZCAPLUS

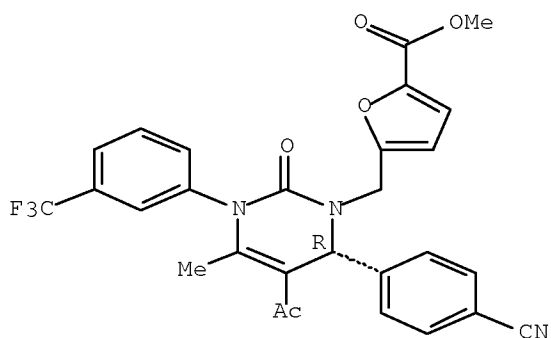
CN 2-Furancarboxylic acid, 5-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



RN 864150-57-2 ZCAPLUS

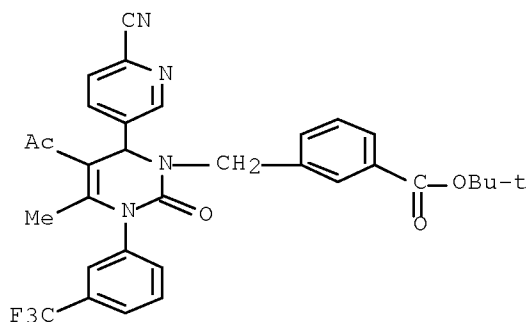
CN 2-Furancarboxylic acid, 5-[[[(6R)-5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



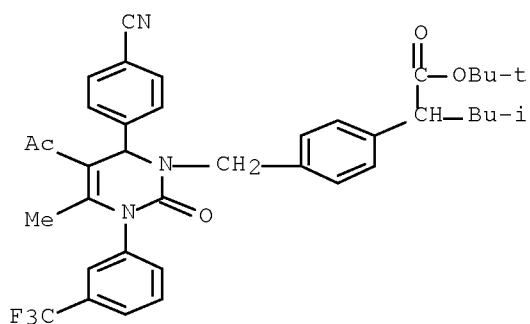
RN 864150-58-3 ZCAPLUS

CN Benzoic acid, 3-[[[5-acetyl-6-(6-cyano-3-pyridinyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



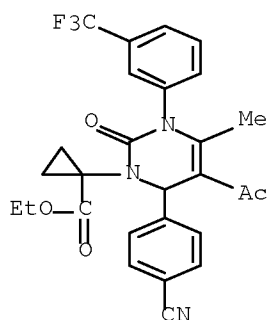
RN 864150-59-4 ZCAPLUS

CN Benzeneacetic acid, 4-[[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- α -(2-methylpropyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



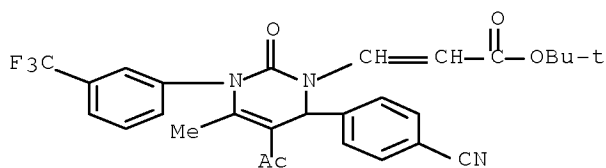
RN 864150-60-7 ZCAPLUS

CN Cyclopropanecarboxylic acid, 1-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]-, ethyl ester (CA INDEX NAME)



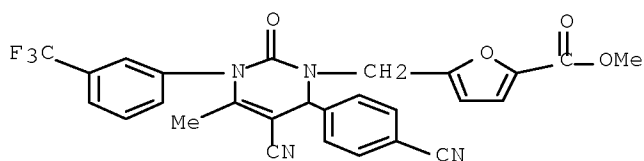
RN 864150-61-8 ZCAPLUS

CN 2-Propenoic acid, 3-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



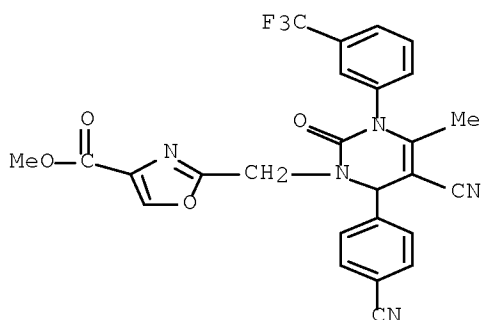
RN 864150-62-9 ZCAPLUS

CN 2-Furancarboxylic acid, 5-[[5-cyano-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



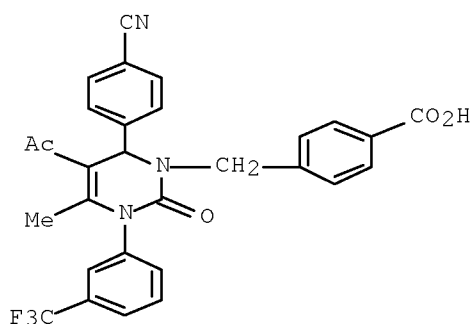
RN 864150-63-0 ZCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[5-cyano-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



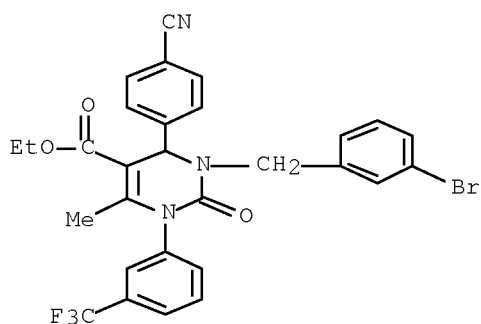
RN 864150-64-1 ZCAPLUS

CN Benzoic acid, 4-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



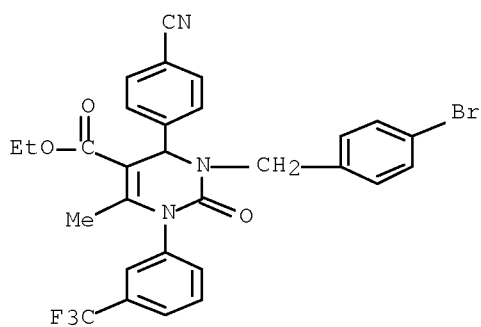
RN 864150-81-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[(3-bromophenyl)methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 864150-82-3 ZCAPLUS

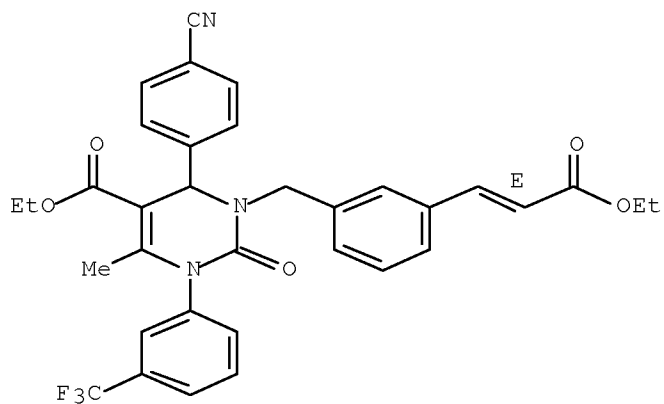
CN 5-Pyrimidinecarboxylic acid, 3-[(4-bromophenyl)methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 864150-83-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[[3-[(1E)-3-ethoxy-3-oxo-1-propen-1-yl]phenyl]methyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

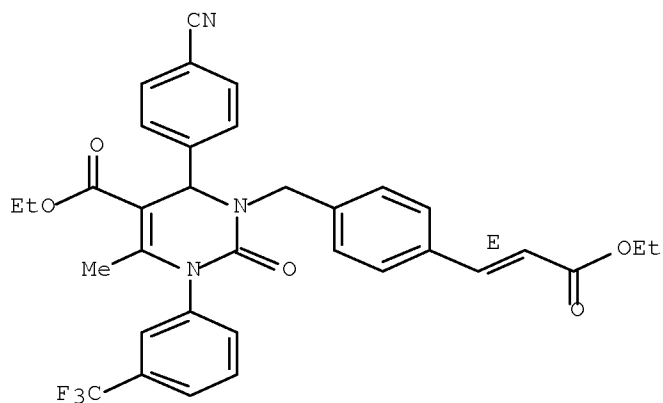
Double bond geometry as shown.



RN 864150-86-7 ZCAPLUS

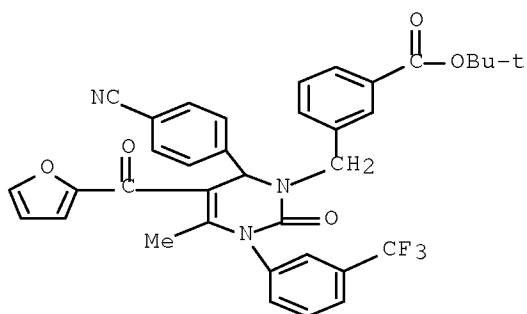
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[[4-[(1E)-3-ethoxy-3-oxo-1-propen-1-yl]phenyl]methyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

Double bond geometry as shown.



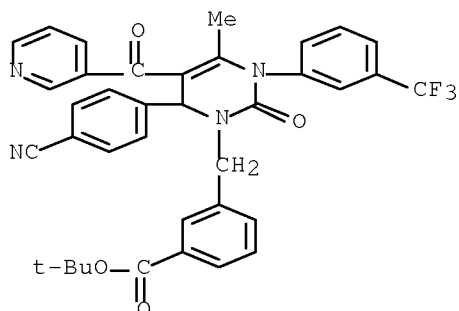
RN 864150-89-0 ZCAPLUS

CN Benzoic acid, 3-[[6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



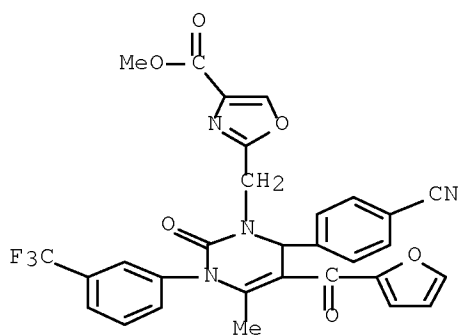
RN 864150-93-6 ZCAPLUS

CN Benzoic acid, 3-[[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(3-pyridinylcarbonyl)-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



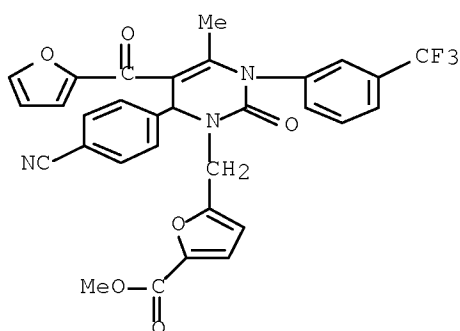
RN 864150-95-8 ZCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



RN 864150-97-0 ZCAPLUS

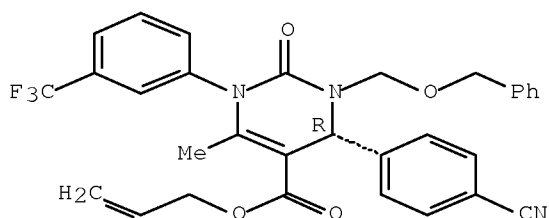
CN 2-Furancarboxylic acid, 5-[[6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



RN 864151-03-1 ZCAPLUS

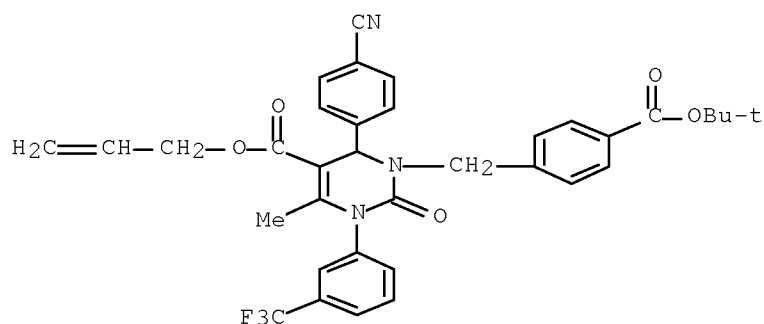
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-[(phenylmethoxy)methyl]-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.



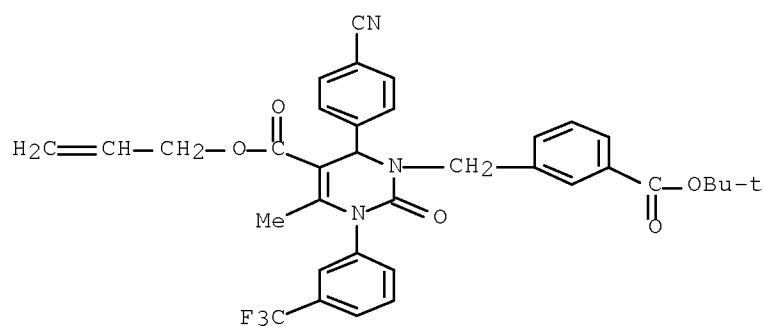
RN 864151-05-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[[4-[(1,1-dimethylethoxy)carbonyl]phenyl]methyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



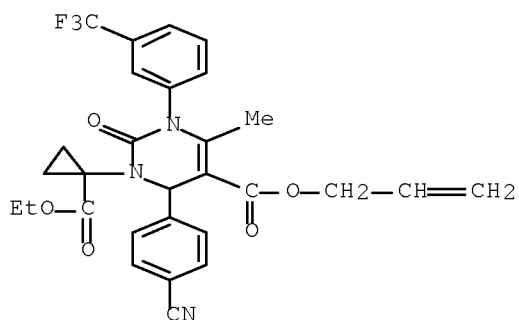
RN 864151-06-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[[3-[(1,1-dimethylethoxy)carbonyl]phenyl]methyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



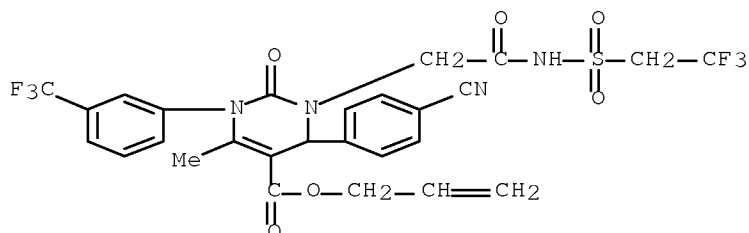
RN 864151-07-5 ZCAPLUS

CN 5(2H)-Pyrimidinecarboxylic acid, 6-(4-cyanophenyl)-1-[1-(ethoxycarbonyl)cyclopropyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



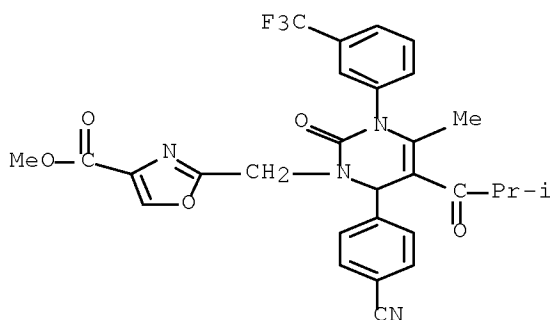
RN 864151-12-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-[2-oxo-2-[(2,2,2-trifluoroethyl)sulfonyl]amino]ethyl]-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



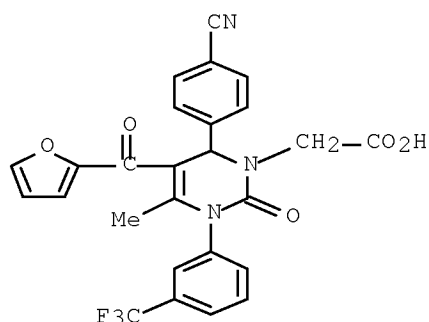
RN 864151-29-1 ZCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(2-methyl-1-oxopropyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



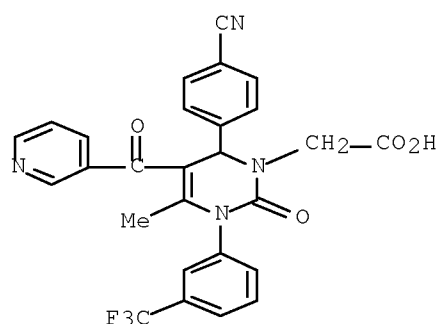
RN 864151-50-8 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864151-51-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(3-pyridinylcarbonyl)-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



IT 864150-65-2P 864150-66-3P 864150-67-4P
 864150-68-5P 864150-69-6P 864150-70-9P
 864150-71-0P 864150-72-1P 864150-73-2P
 864150-74-3P 864150-75-4P 864150-76-5P
 864150-77-6P 864150-78-7P 864150-79-8P
 864150-80-1P 864150-84-5P 864150-85-6P
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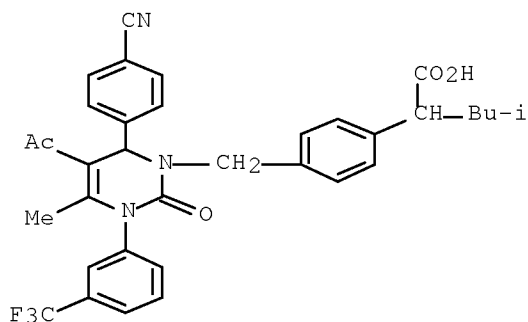
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of tetrasubstituted pyrimidin-2-ones as human neutrophil elastase inhibitors)

RN 864150-65-2 ZCAPLUS

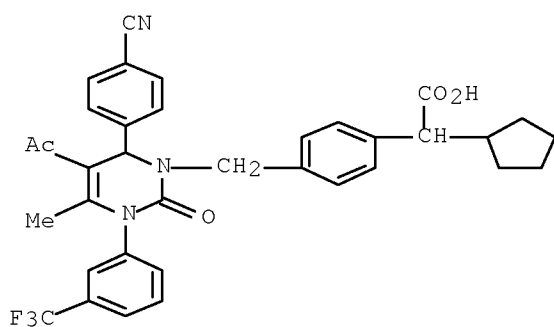
CN Benzeneacetic acid, 4-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-

oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl)methyl]- α -(2-methylpropyl)- (CA INDEX NAME)



RN 864150-66-3 ZCAPLUS

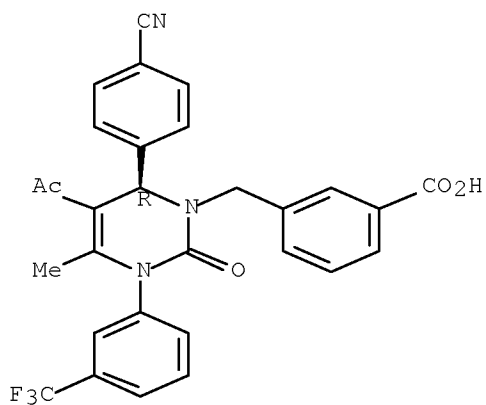
CN Benzeneacetic acid, 4-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- α -cyclopentyl- (CA INDEX NAME)



RN 864150-67-4 ZCAPLUS

CN Benzoic acid, 3-[[[(6R)-5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-2-cyclopentyl] (CA INDEX NAME)

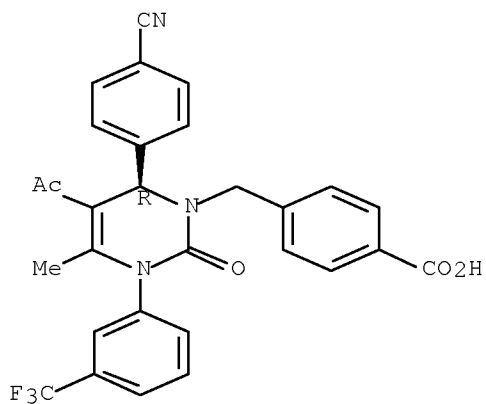
Absolute stereochemistry.



RN 864150-68-5 ZCAPLUS

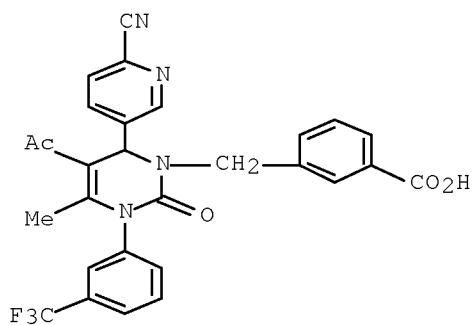
CN Benzoic acid, 4-[[(6R)-5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.



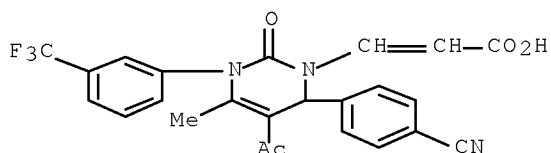
RN 864150-69-6 ZCAPLUS

CN Benzoic acid, 3-[[5-acetyl-6-(6-cyano-3-pyridinyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



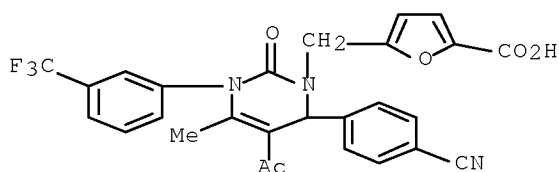
RN 864150-70-9 ZCAPLUS

CN 2-Propenoic acid, 3-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]- (CA INDEX NAME)



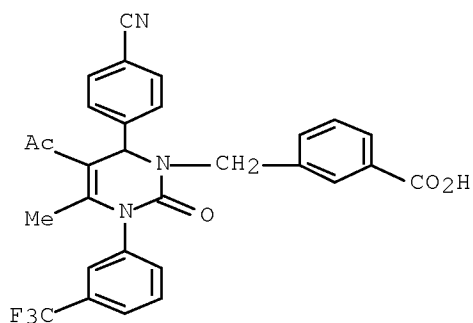
RN 864150-71-0 ZCAPLUS

CN 2-Furancarboxylic acid, 5-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



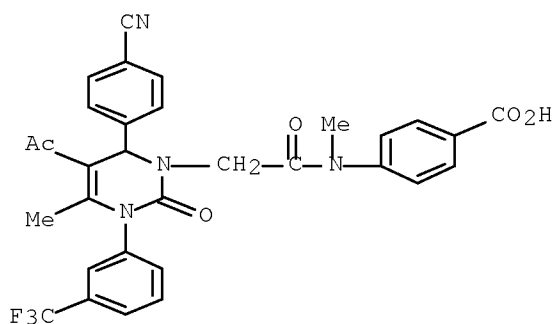
RN 864150-72-1 ZCAPLUS

CN Benzoic acid, 3-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



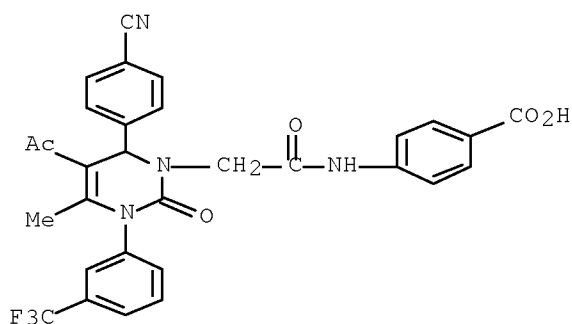
RN 864150-73-2 ZCAPLUS

CN Benzoic acid, 4-[[2-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]methylamino]- (CA INDEX NAME)



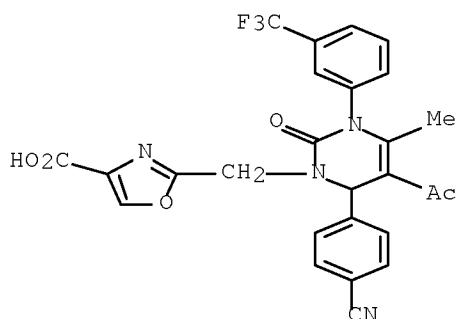
RN 864150-74-3 ZCAPLUS

CN Benzoic acid, 4-[[2-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]- (CA INDEX NAME)



RN 864150-75-4 ZCAPLUS

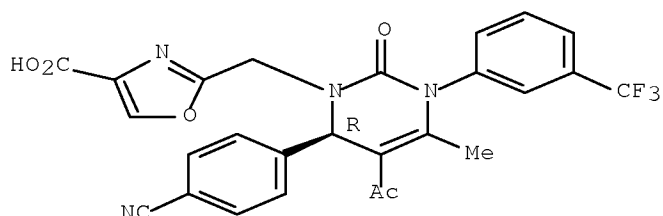
CN 4-Oxazolecarboxylic acid, 2-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



RN 864150-76-5 ZCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[[(6R)-5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)

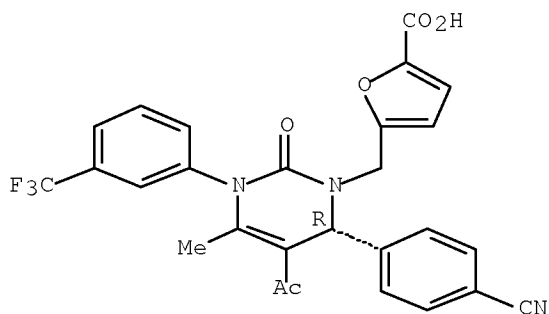
Absolute stereochemistry.



RN 864150-77-6 ZCAPLUS

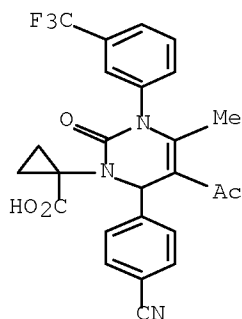
CN 2-Furancarboxylic acid, 5-[[(6R)-5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 864150-78-7 ZCAPLUS

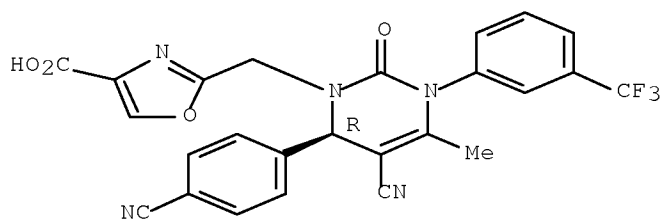
CN Cyclopropanecarboxylic acid, 1-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]- (CA INDEX NAME)



RN 864150-79-8 ZCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[(6R)-5-cyano-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)

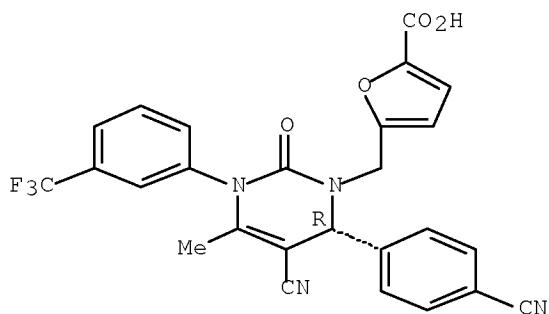
Absolute stereochemistry.



RN 864150-80-1 ZCAPLUS

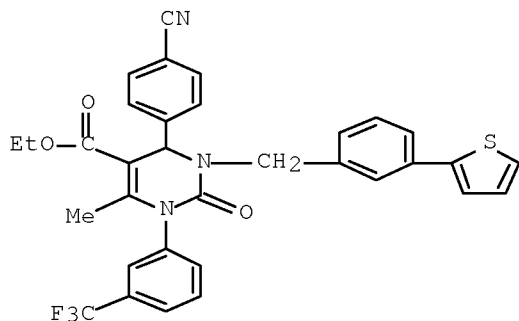
CN 2-Furancarboxylic acid, 5-[[(6R)-5-cyano-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 864150-84-5 ZCAPLUS

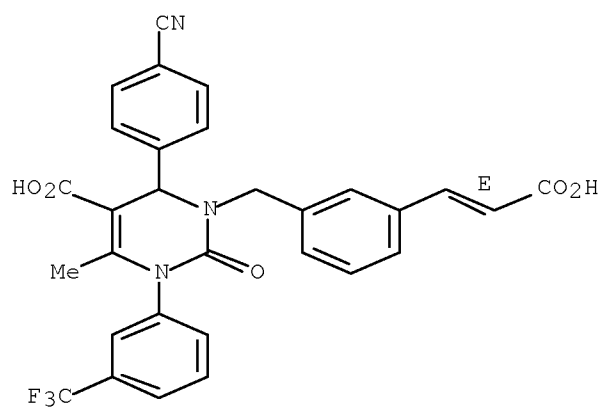
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-[[3-(2-thienyl)phenyl]methyl]-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 864150-85-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[[3-[(1E)-2-carboxyethenyl]phenyl]methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

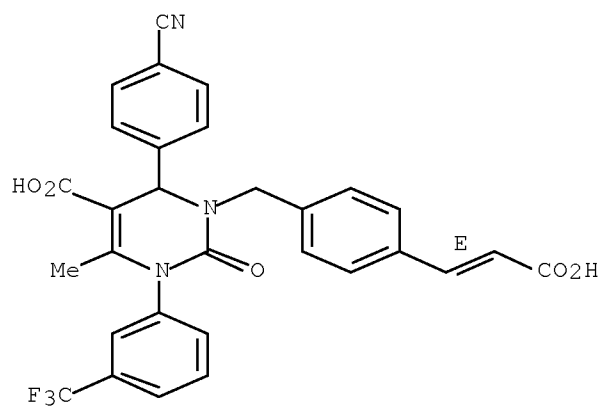
Double bond geometry as shown.



RN 864150-87-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[[4-[(1E)-2-carboxyethenyl]phenyl]methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

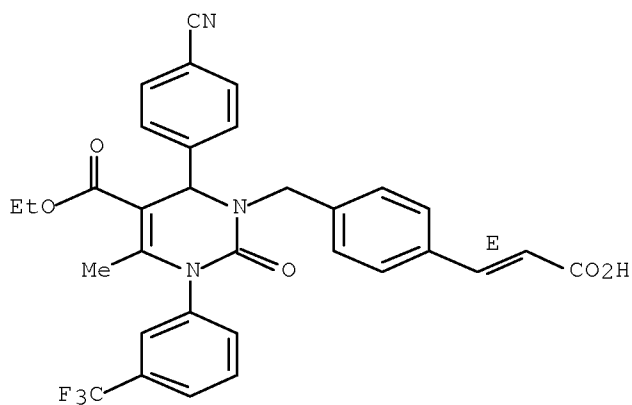
Double bond geometry as shown.



RN 864150-88-9 ZCAPLUS

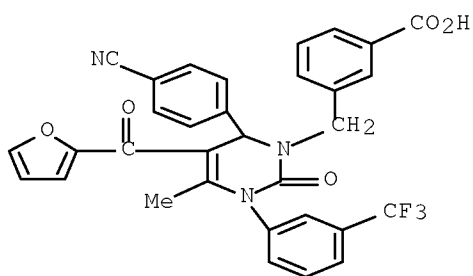
CN 5-Pyrimidinecarboxylic acid, 3-[[4-[(1E)-2-carboxyethenyl]phenyl]methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 5-ethyl ester (CA INDEX NAME)

Double bond geometry as shown.



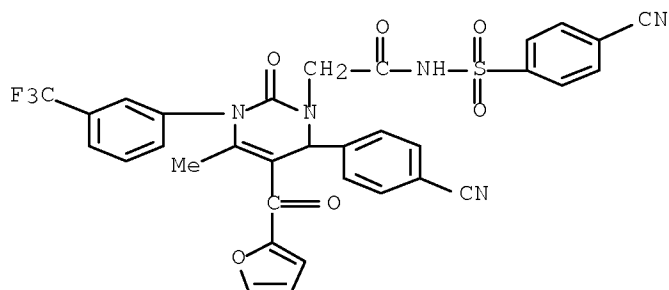
RN 864150-90-3 ZCAPLUS

CN Benzoic acid, 3-[[6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



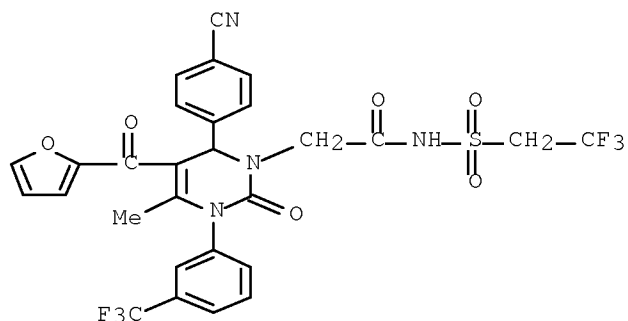
RN 864150-91-4 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-N-[(4-cyanophenyl)sulfonyl]-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



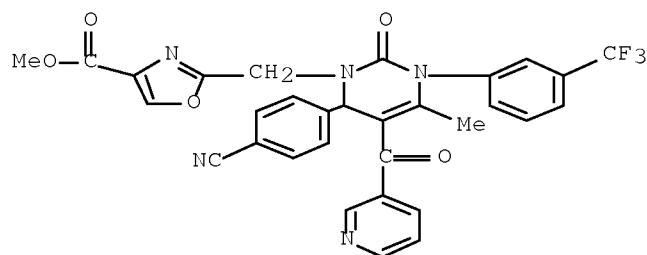
RN 864150-92-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-N-[(2,2,2-trifluoroethyl)sulfonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



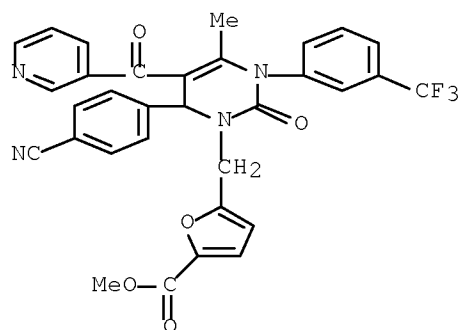
RN 864150-94-7 ZCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(3-pyridinylcarbonyl)-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



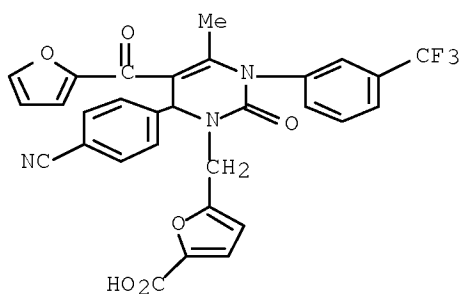
RN 864150-96-9 ZCAPLUS

CN 2-Furancarboxylic acid, 5-[[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(3-pyridinylcarbonyl)-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



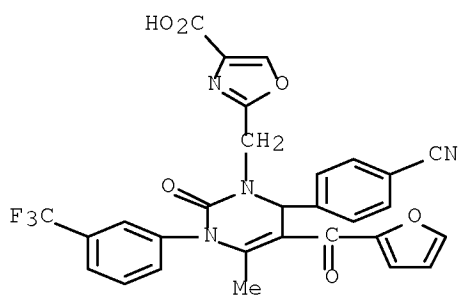
RN 864150-98-1 ZCAPLUS

CN 2-Furancarboxylic acid, 5-[[6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



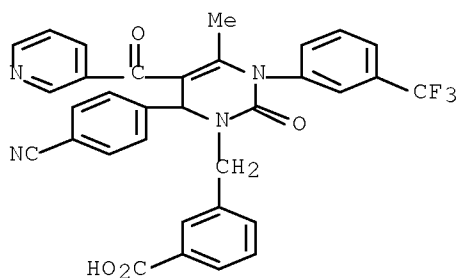
RN 864150-99-2 ZCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



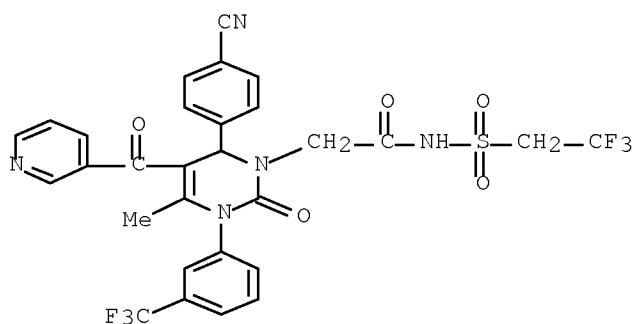
RN 864151-00-8 ZCAPLUS

CN Benzoic acid, 3-[[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(3-pyridinylcarbonyl)-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



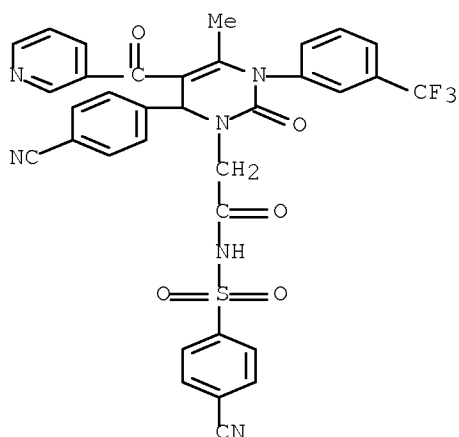
RN 864151-01-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(3-pyridinylcarbonyl)-N-[(2,2,2-trifluoroethyl)sulfonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864151-02-0 ZCAPLUS

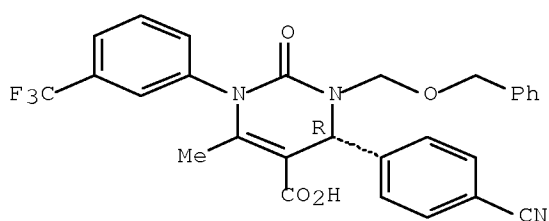
CN 1(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-N-[(4-cyanophenyl)sulfonyl]-3,6-dihydro-4-methyl-2-oxo-5-(3-pyridinylcarbonyl)-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864151-04-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-[(phenylmethoxy)methyl]-1-[3-(trifluoromethyl)phenyl]-, (4R)- (CA INDEX NAME)

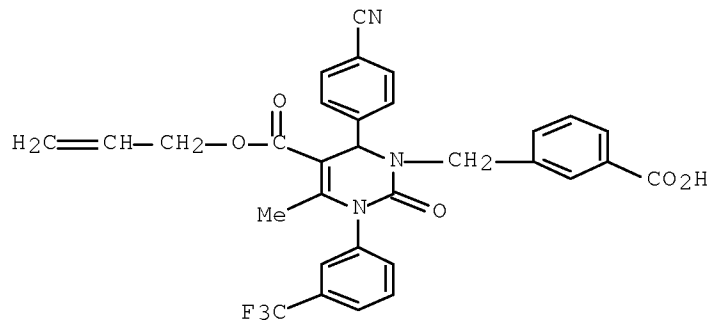
Absolute stereochemistry.



RN 864151-08-6 ZCAPLUS

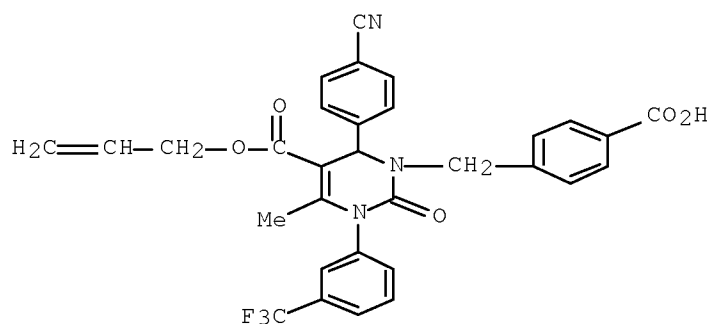
CN 5-Pyrimidinecarboxylic acid, 3-[(3-carboxyphenyl)methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R)- (CA INDEX NAME)

5-(2-propen-1-yl) ester (CA INDEX NAME)



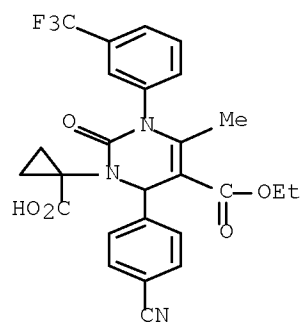
RN 864151-09-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[(4-carboxyphenyl)methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 5-(2-propen-1-yl) ester (CA INDEX NAME)



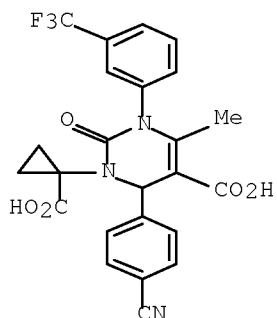
RN 864151-10-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(1-carboxycyclopropyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 5-ethyl ester (9CI) (CA INDEX NAME)



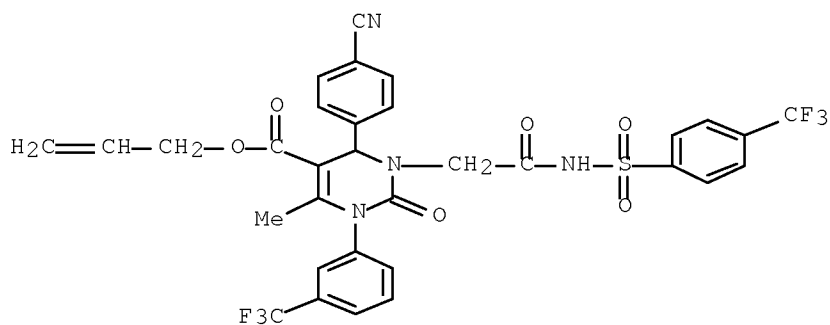
RN 864151-11-1 ZCAPLUS

CN 5(2H)-Pyrimidinecarboxylic acid, 1-(1-carboxycyclopropyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



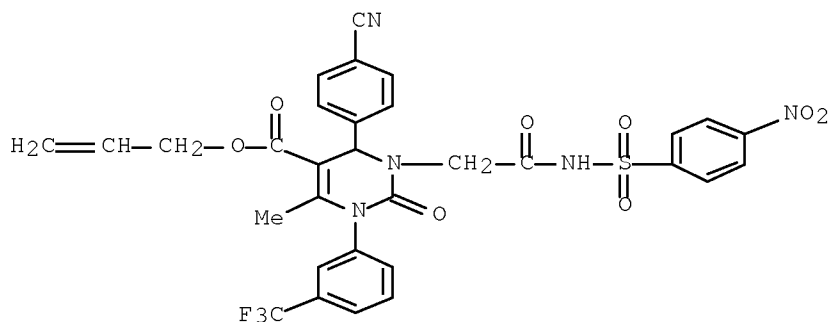
RN 864151-13-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-[2-oxo-2-[[[4-(trifluoromethyl)phenyl]sulfonyl]amino]ethyl]-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



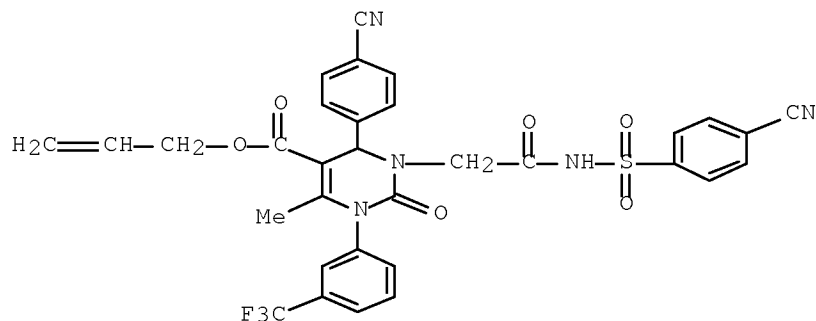
RN 864151-14-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[2-[[[4-(nitrophenyl)sulfonyl]amino]-2-oxoethyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



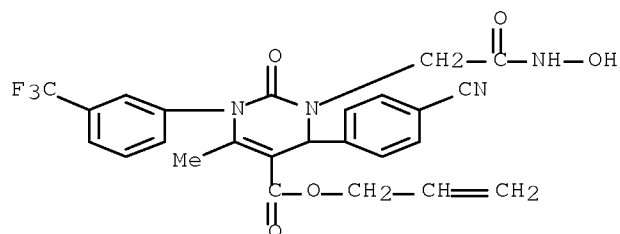
RN 864151-15-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[4-cyanophenyl)sulfonyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



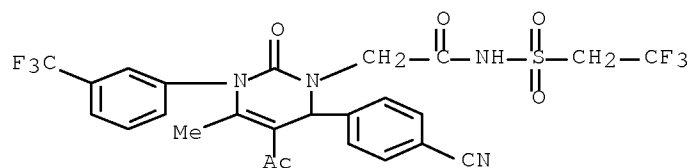
RN 864151-16-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[2-(hydroxyamino)-2-oxoethyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



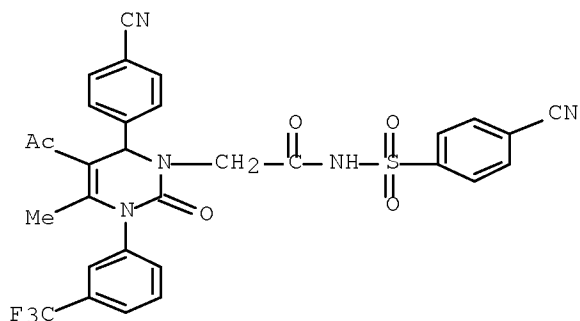
RN 864151-17-7 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-N-[(2,2,2-trifluoroethyl)sulfonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864151-18-8 ZCAPLUS

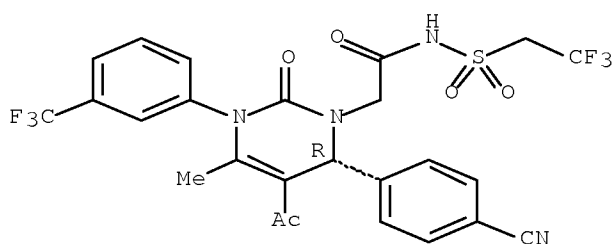
CN 1(2H)-Pyrimidineacetamide, 5-acetyl-6-(4-cyanophenyl)-N-[(4-cyanophenyl)sulfonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864151-19-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-N-[(2,2,2-trifluoroethyl)sulfonyl]-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

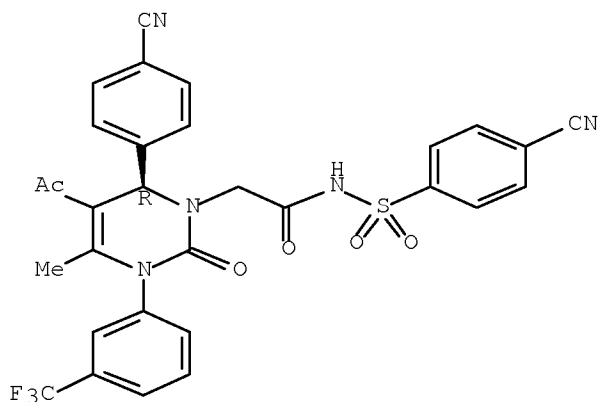
Absolute stereochemistry.



RN 864151-20-2 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 5-acetyl-6-(4-cyanophenyl)-N-[(4-cyanophenyl)sulfonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

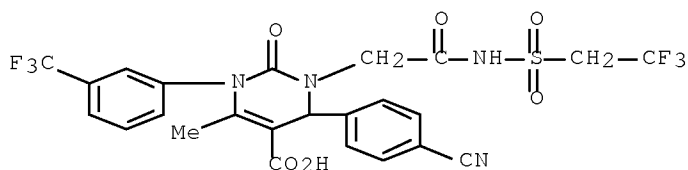
Absolute stereochemistry.



RN 864151-21-3 ZCAPLUS

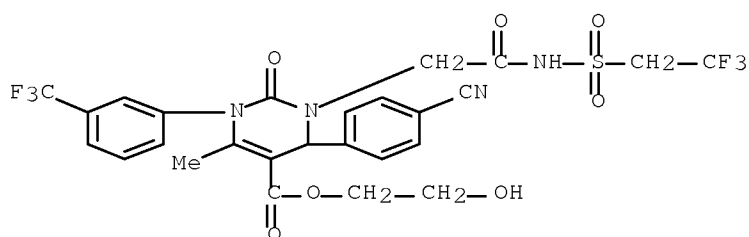
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-N-[(2,2,2-trifluoroethyl)sulfonyl]-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

2-oxo-3-[2-oxo-2-[[(2,2,2-trifluoroethyl) sulfonyl] amino]ethyl]-1-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



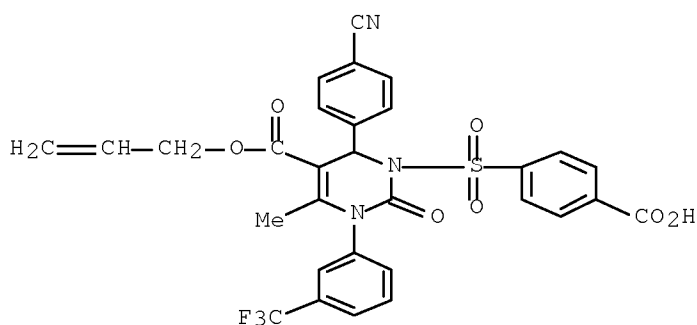
RN 864151-22-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-[2-oxo-2-[[(2,2,2-trifluoroethyl) sulfonyl] amino]ethyl]-1-[3-(trifluoromethyl)phenyl]-, 2-hydroxyethyl ester (CA INDEX NAME)



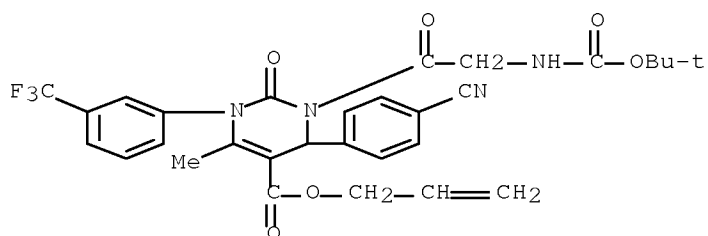
RN 864151-23-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[(4-carboxyphenyl) sulfonyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 5-(2-propen-1-yl) ester (CA INDEX NAME)



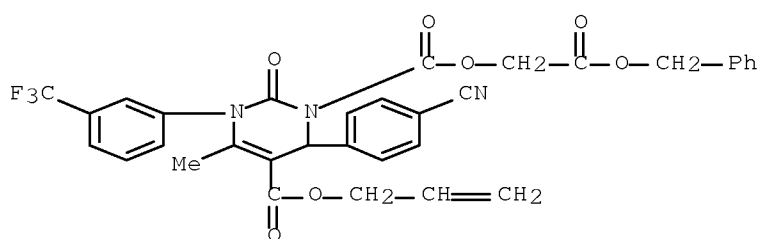
RN 864151-24-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[(1,1-dimethylethoxy) carbonyl] amino]acetyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



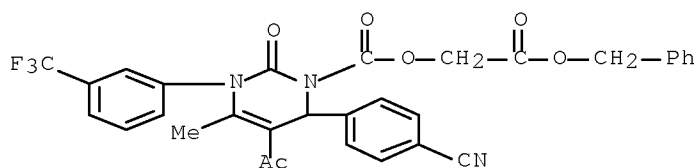
RN 864151-25-7 ZCAPLUS

CN 1,5(2H)-Pyrimidinedicarboxylic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1-[2-oxo-2-(phenylmethoxy)ethyl] 5-(2-propen-1-yl) ester (CA INDEX NAME)



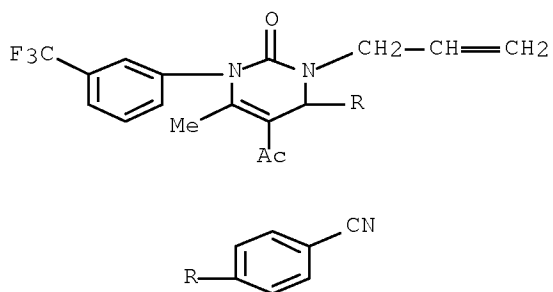
RN 864151-26-8 ZCAPLUS

CN 1(2H)-Pyrimidinecarboxylic acid, 5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 2-oxo-2-(phenylmethoxy)ethyl ester (CA INDEX NAME)



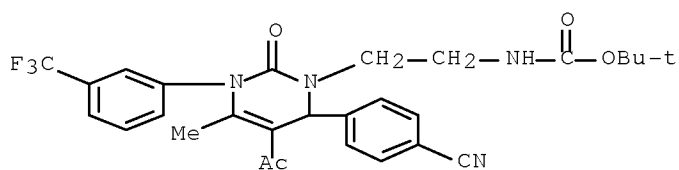
RN 864151-27-9 ZCAPLUS

CN Benzonitrile, 4-[5-acetyl-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(2-propen-1-yl)-1-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]- (CA INDEX NAME)



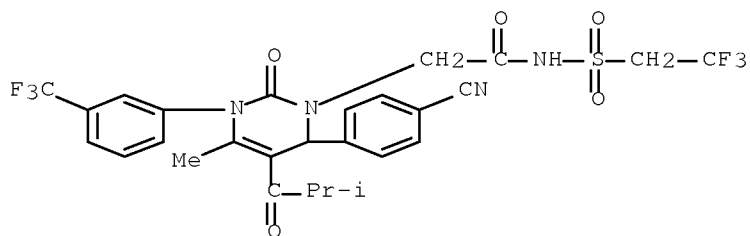
RN 864151-28-0 ZCAPLUS

CN Carbamic acid, [2-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



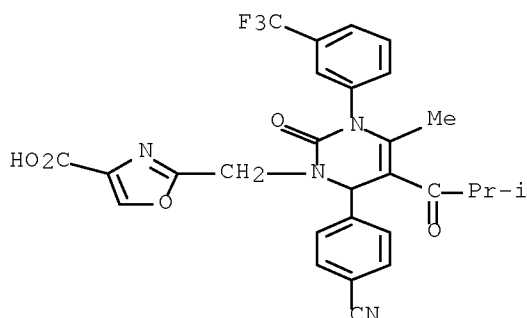
RN 864151-30-4 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(2-methyl-1-oxopropyl)-2-oxo-N-[(2,2,2-trifluoroethyl)sulfonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864151-31-5 ZCAPLUS

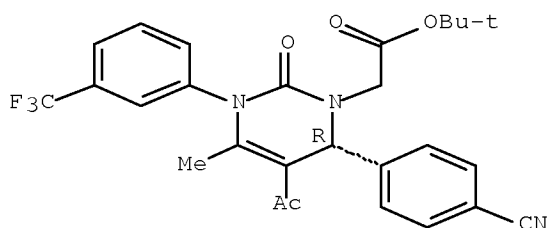
CN 4-Oxazolecarboxylic acid, 2-[[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(2-methyl-1-oxopropyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



RN 864151-49-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, (6R)- (CA INDEX NAME)

Absolute stereochemistry.



IT 864151-38-2P 864151-39-3P 864151-40-6P

864151-41-7P 864151-42-8P 864151-43-9P

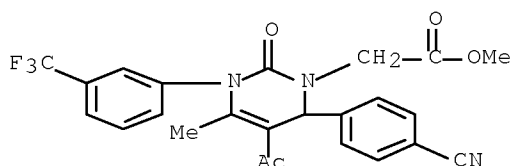
864151-44-0P 864151-45-1P 864151-46-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tetrasubstituted pyrimidin-2-ones as human neutrophil elastase inhibitors)

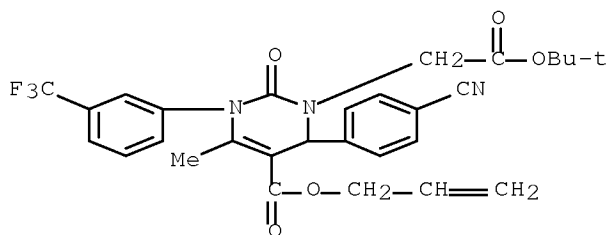
RN 864151-38-2 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, methyl ester (CA INDEX NAME)



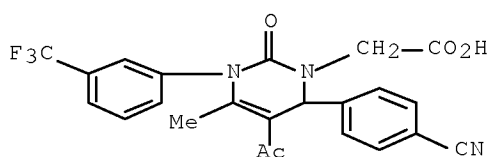
RN 864151-39-3 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



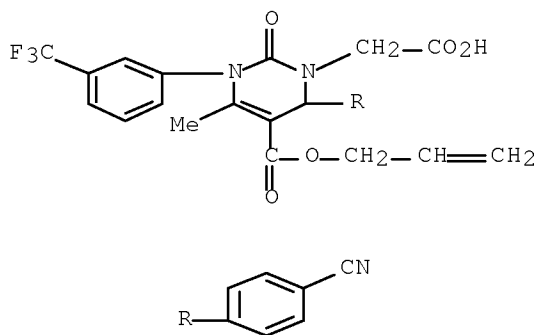
RN 864151-40-6 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864151-41-7 ZCAPLUS

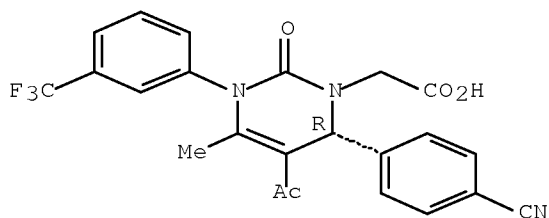
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864151-42-8 ZCAPLUS

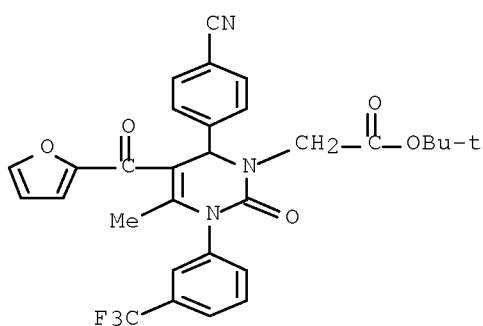
CN 1(2H)-Pyrimidineacetic acid, 5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.



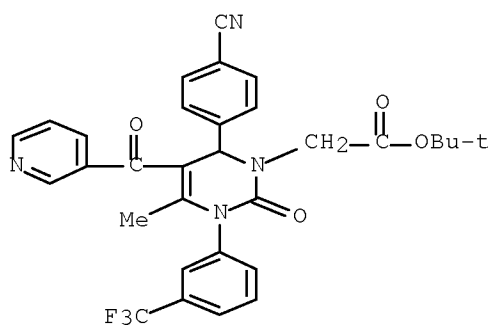
RN 864151-43-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



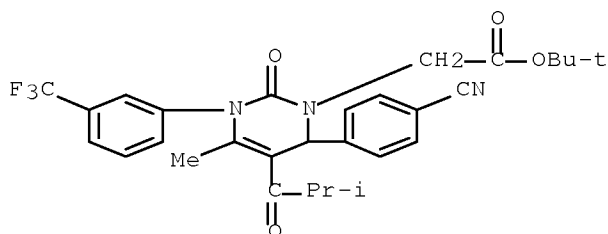
RN 864151-44-0 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(3-pyridinylcarbonyl)-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



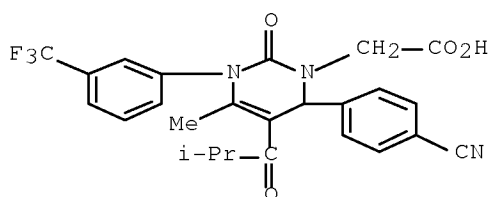
RN 864151-45-1 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(2-methyl-1-oxopropyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864151-46-2 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(2-methyl-1-oxopropyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L6 ANSWER 7 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:253147 ZCAPLUS Full-text

DOCUMENT NUMBER: 140:287406

TITLE: Preparation of pyrimidinones as human neutrophil elastase (HNE) inhibitors

INVENTOR(S): Gielen, Heike; Li, Volkhart; Rosentreter, Ulrich; Schlemmer, Karl-heinz; Allerheiligen, Swen; Telan, Leila; Baerfacker, Lars; Keldenich, Joerg; Fitzgerald, Mary F.; Nash, Kevin; Albrecht, Barbara; Meurer, Dirk

PATENT ASSIGNEE(S): Bayer Healthcare Ag, Germany

SOURCE: PCT Int. Appl., 121 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

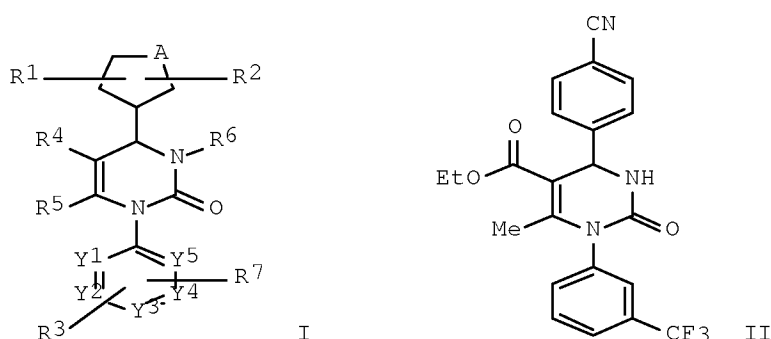
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
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| WO 2004024700 | A1 | 20040325 | WO 2003-EP9525 | 20030828 |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | |
| RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
| GB 2392910 | A | 20040317 | GB 2003-15870 | 20030707 |
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| | | | | |
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| BR 2003014186 | A | 20050809 | BR 2003-14186 | 20030828 |
| JP 2006507355 | T | 20060302 | JP 2004-571738 | 20030828 |
| NZ 538670 | A | 20070126 | NZ 2003-538670 | 20030828 |
| MX 2005PA02644 | A | 20050920 | MX 2005-PA2644 | 20050309 |
| NO 2005001726 | A | 20050407 | NO 2005-1726 | 20050407 |
| US 20060160801 | A1 | 20060720 | US 2005-527391 | 20051021 |
| PRIORITY APPLN. INFO.: | | | GB 2002-20962 | A 20020910 |
| | | | GB 2002-26609 | A 20021114 |
| | | | GB 2003-15870 | A 20030707 |
| | | | WO 2003-EP9525 | W 20030828 |
| OTHER SOURCE(S): | | | MARPAT 140:287406 | |
| GI | | | | |

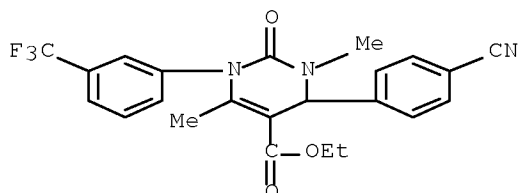


- AB Title compds. I [wherein A = hetero/aryl; R1, R2, R3 = independently H, halo, NO2, CN, OH and derivs., (un)substituted alkyl, R4 = CN, trifluoromethylcarbonyl, alkenoxycarbonyl, hydroxycarbonyl, aryl/alkylaminocarbonyl, (un)substituted heteroarylcarbonyl, heterocyclylcarbonyl, heteroaryl, heterocyclyl, alkylcarbonyl, alkoxycarbonyl, mono- and dialkylaminocarbonyl; R5 = NH2, (un)substituted alkyl; R6 = H, formyl, N-(alkylsulfonyl)/N-(alkylsulfonyl)-N- (alkyl)/aminocarbonyl, heteroarylcarbonyl, heterocyclylcarbonyl, cycloalkylcarbonyl, (un)substituted alkyl, mono- and dialkylaminocarbonyl, alkylcarbonyl, alkoxycarbonyl, heteroaryl, heterocyclyl, etc.; R7 = halo, NO2, CN, OH, (un)substituted alkyl, alkoxy; Y1, Y2, Y3, Y4, Y5 = independently CH or N; and their salts, hydrates, and/or solvates, and their tautomeric forms] were prepared as human neutrophil elastase (HNE) inhibitors. For example, II was prepared, in 91% yield, by cyclocondensation of N-[3-(trifluoromethyl)phenyl]urea with 4-cyanobenzaldehyde and Et 3-oxobutanoate. In an in vitro assay, II displayed an IC50 value of 8 nM for HNE inhibition. Thus, I are useful for treatment of acute and chronic inflammation, ischemic and remodelling processes, in particular chronic obstructive pulmonary diseases.
- IT 671775-98-7P, Ethyl 4-(4-cyanophenyl)-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate
 671776-27-5P 671776-58-2P, 4-(4-Cyanophenyl)-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-1,2,3,4-tetrahydro-5-pyrimidinecarboxylic acid
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(human neutrophil elastase inhibitor; preparation of pyrimidinones as human neutrophil elastase inhibitors)

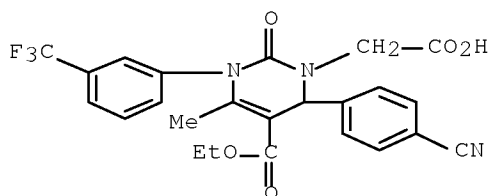
RN 671775-98-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



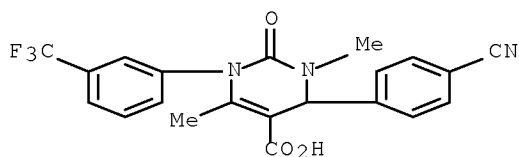
RN 671776-27-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 671776-58-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



IT 671775-94-3P, Ethyl 4-(4-cyanophenyl)-3-formyl-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate
 671775-99-8P, Ethyl 3-acetyl-4-(4-cyanophenyl)-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate
 671776-00-4P, Diethyl 6-(4-cyanophenyl)-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-3,6-dihydro-1,5(2H)-pyrimidinedicarboxylate
 671776-14-0P 671776-15-1P 671776-16-2P
 671776-17-3P 671776-18-4P 671776-19-5P
 671776-20-8P 671776-21-9P 671776-22-0P
 671776-23-1P 671776-24-2P 671776-25-3P
 671776-26-4P 671776-28-6P 671776-29-7P
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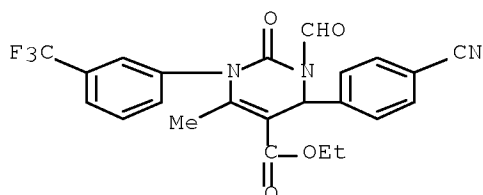
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 671776-43-5P 671776-44-6P 671776-45-7P
 671776-69-5P 671776-70-8P 671776-71-9P
 671776-72-0P 671776-73-1P 671776-74-2P
 671776-75-3P 671776-76-4P 671776-77-5P
 671776-78-6P 671776-79-7P 671776-80-0P
 671776-81-1P 675103-27-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(human neutrophil elastase inhibitor; preparation of pyrimidinones as human neutrophil elastase inhibitors)

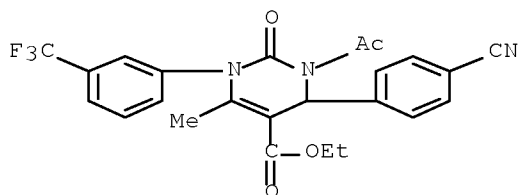
RN 671775-94-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-formyl-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



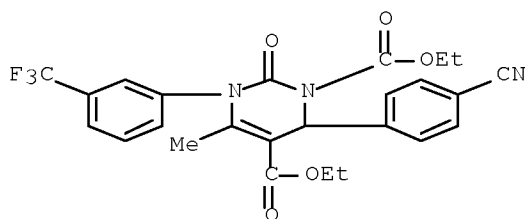
RN 671775-99-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-acetyl-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



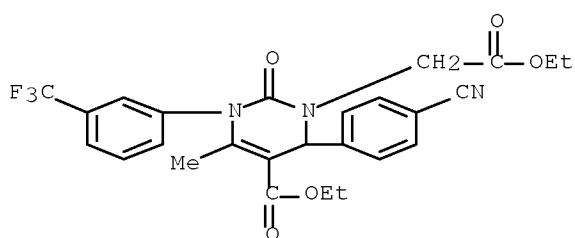
RN 671776-00-4 ZCAPLUS

CN 1,5(2H)-Pyrimidinedicarboxylic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,5-diethyl ester (CA INDEX NAME)



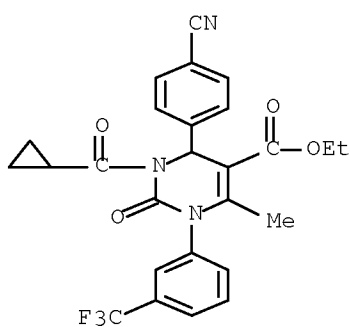
RN 671776-14-0 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



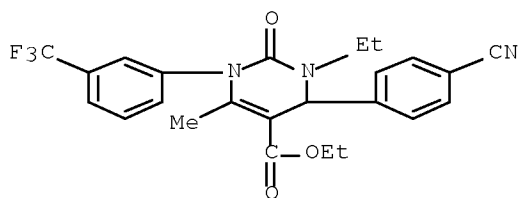
RN 671776-15-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-(cyclopropylcarbonyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



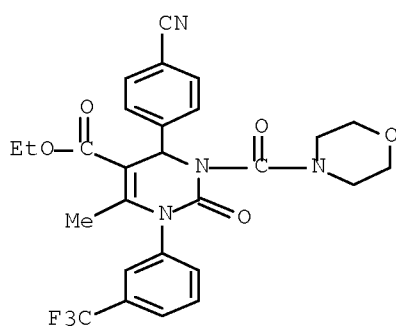
RN 671776-16-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-ethyl-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



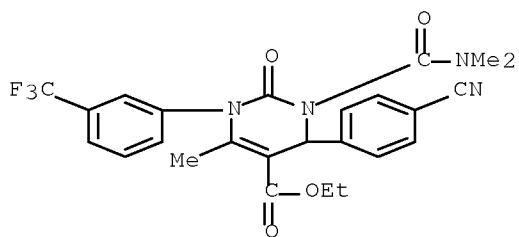
RN 671776-17-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-(4-morpholinylcarbonyl)-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



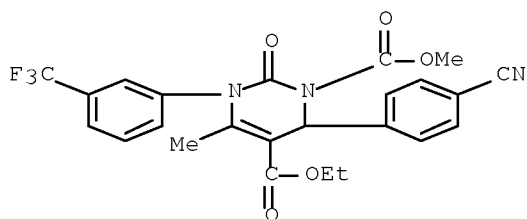
RN 671776-18-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[(dimethylamino)carbonyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



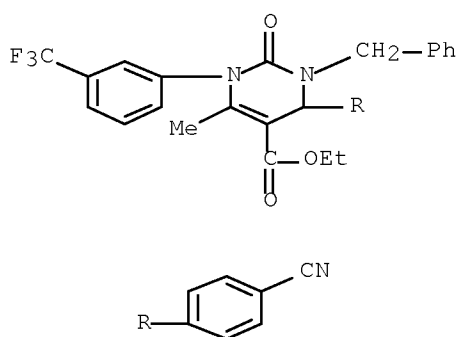
RN 671776-19-5 ZCAPLUS

CN 1,5(2H)-Pyrimidinedicarboxylic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 5-ethyl 1-methyl ester (CA INDEX NAME)



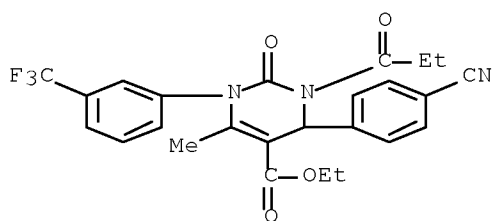
RN 671776-20-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(phenylmethyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



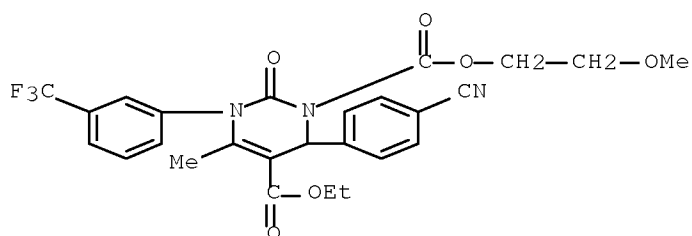
RN 671776-21-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(1-oxopropyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



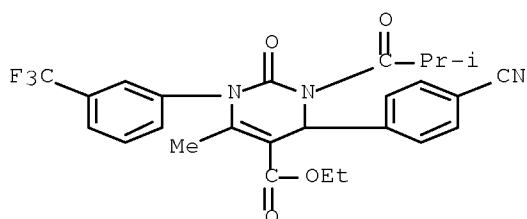
RN 671776-22-0 ZCAPLUS

CN 1,5(2H)-Pyrimidinedicarboxylic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 5-ethyl 1-(2-methoxyethyl) ester (CA INDEX NAME)



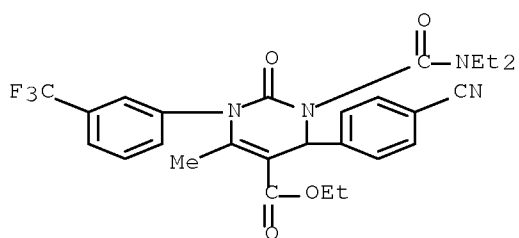
RN 671776-23-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-(2-methyl-1-oxopropyl)-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



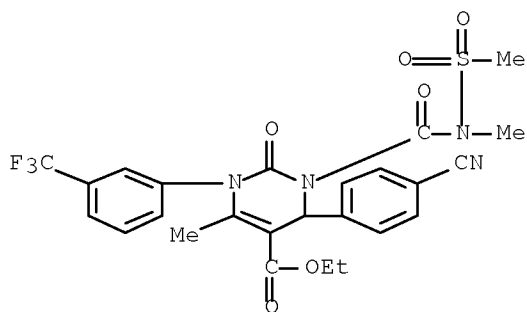
RN 671776-24-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[(diethylamino)carbonyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



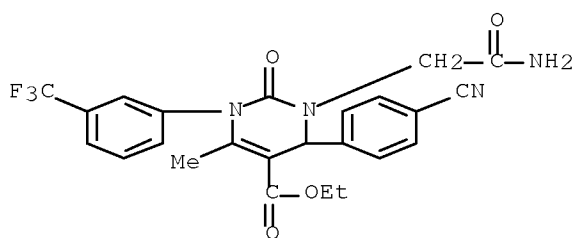
RN 671776-25-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[[methyl(methylsulfonyl)amino]carbonyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



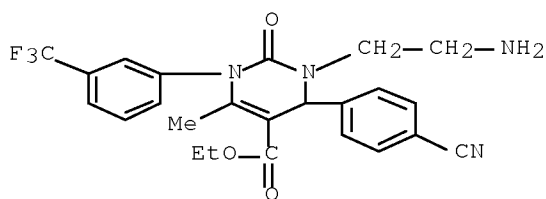
RN 671776-26-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(2-amino-2-oxoethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



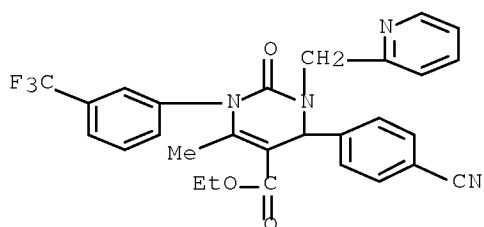
RN 671776-28-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(2-aminoethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



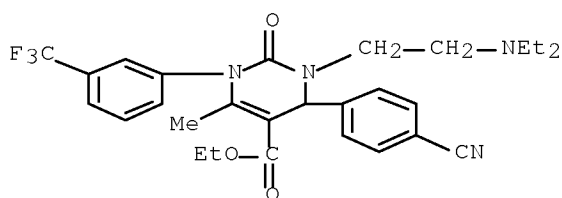
RN 671776-29-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(2-pyridinylmethyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



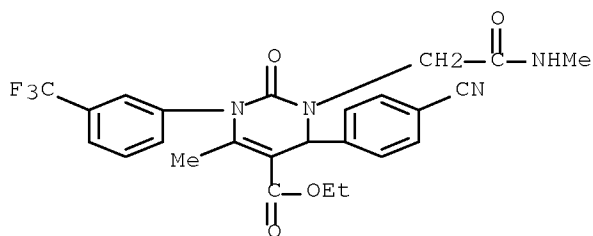
RN 671776-30-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-(diethylamino)ethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



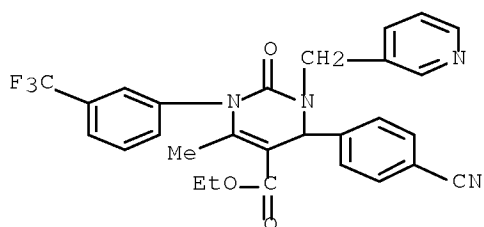
RN 671776-31-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[2-(methylamino)-2-oxoethyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



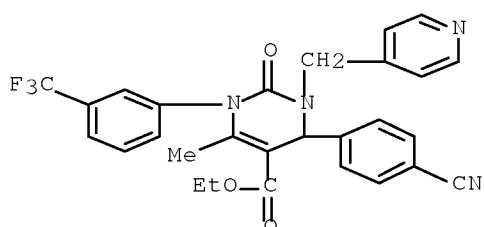
RN 671776-32-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(3-pyridinylmethyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



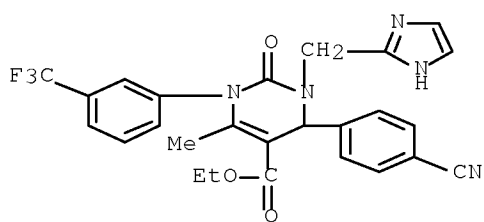
RN 671776-33-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(4-pyridinylmethyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



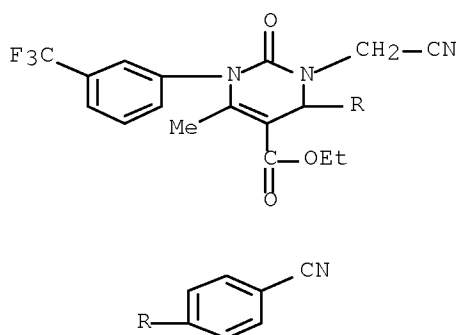
RN 671776-34-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-(1H-imidazol-2-ylmethyl)-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



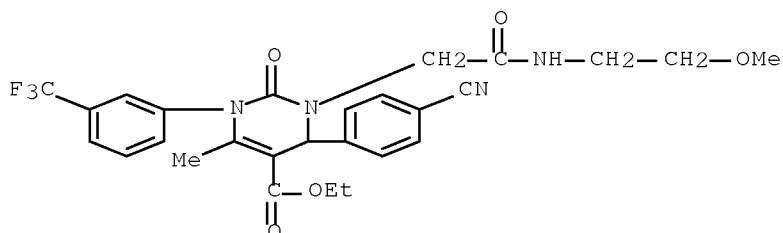
RN 671776-35-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(cyanomethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



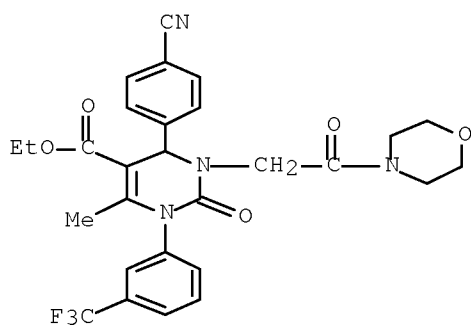
RN 671776-36-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[2-[(2-methoxyethyl)amino]-2-oxoethyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



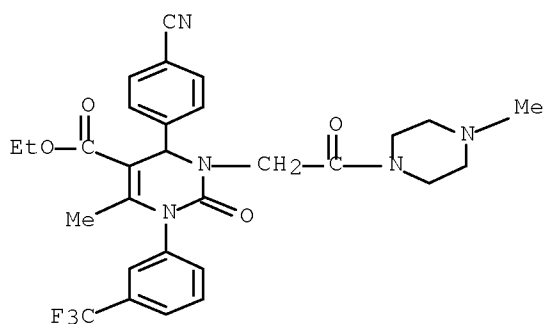
RN 671776-42-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[2-(4-morpholinyl)-2-oxoethyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



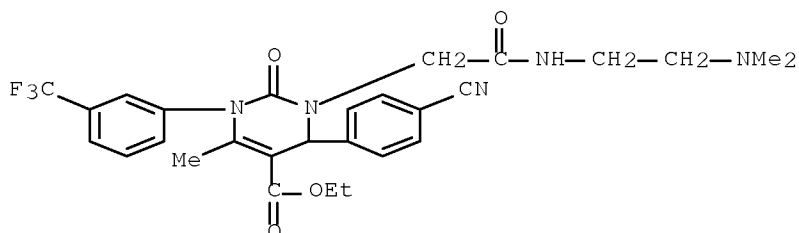
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CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[2-(4-methyl-1-piperazinyl)-2-oxoethyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



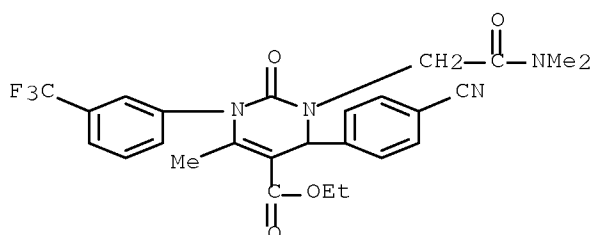
RN 671776-44-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-(dimethylamino)ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



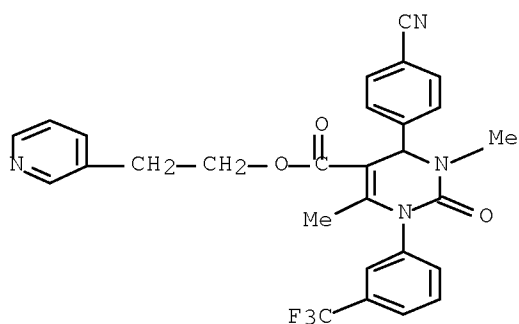
RN 671776-45-7 ZCAPLUS

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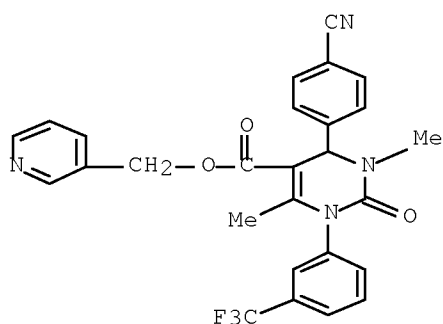
RN 671776-69-5 ZCAPLUS

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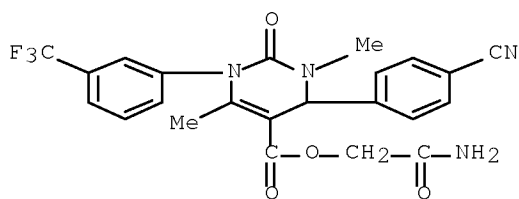
RN 671776-70-8 ZCAPLUS

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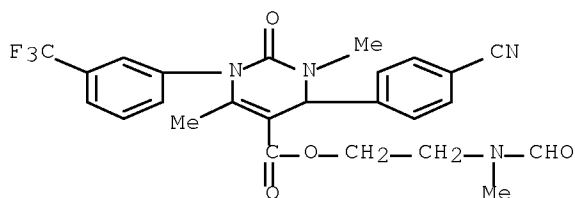
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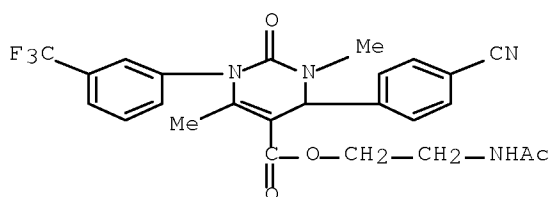
RN 671776-72-0 ZCAPLUS

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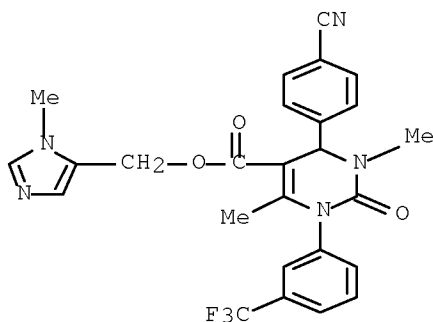
RN 671776-73-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(acetamino)ethyl ester (CA INDEX NAME)



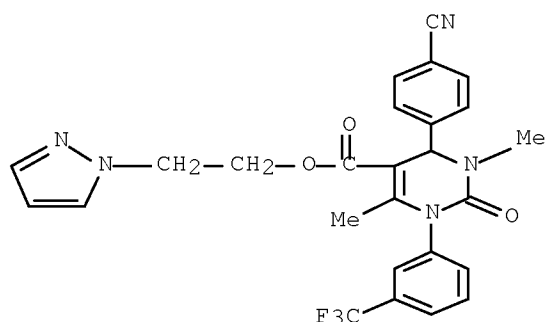
RN 671776-74-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (1-methyl-1H-imidazol-5-yl)methyl ester (CA INDEX NAME)



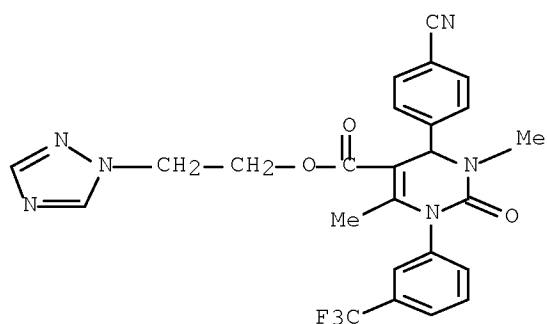
RN 671776-75-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(1H-pyrazol-1-yl)ethyl ester (CA INDEX NAME)



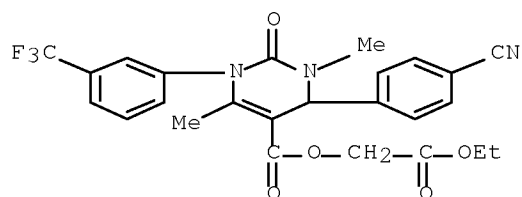
RN 671776-76-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(1H-1,2,4-triazol-1-yl)ethyl ester (CA INDEX NAME)



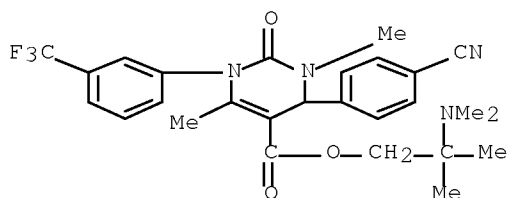
RN 671776-77-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-ethoxy-2-oxoethyl ester (CA INDEX NAME)



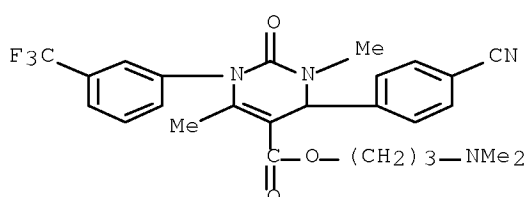
RN 671776-78-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(dimethylamino)-2-methylpropyl ester (CA INDEX NAME)



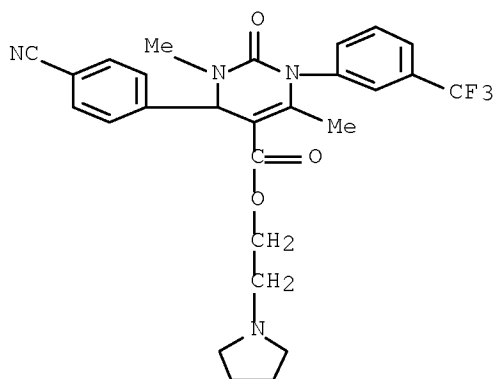
RN 671776-79-7 ZCAPLUS

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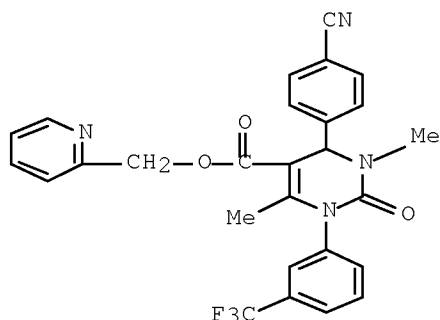
RN 671776-80-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(1-pyrrolidinyl)ethyl ester (CA INDEX NAME)



RN 671776-81-1 ZCAPLUS

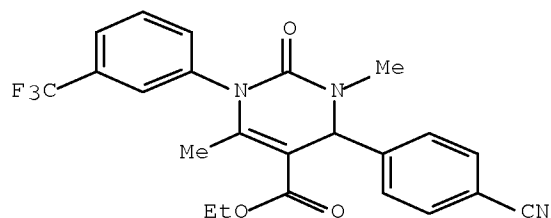
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-pyridinylmethyl ester (CA INDEX NAME)



RN 675103-27-2 ZCAPLUS

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Rotation (-).



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ACCESSION NUMBER: 2004:213317 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 140:253573

TITLE: Preparation of 2-oxopyrimidines as human leukocyte elastase (HNE) inhibitors

INVENTOR(S): Gielen, Heike; Li, Volkhart Min-jian; Rosentreter, Ulrich; Schlemmer, Karl-heinz; Allerheiligen, Swen; Telan, Leila; Baerfacker, Lars; Keldenich, Joerg; Albrecht, Barbara; Meurer, Dirk; Fitzgerald, Mary; Nash, Kevin

PATENT ASSIGNEE(S): Bayer Ag, Germany

SOURCE: Brit. UK Pat. Appl., 117 pp.

CODEN: BAXXDU

DOCUMENT TYPE: Patent

LANGUAGE: English

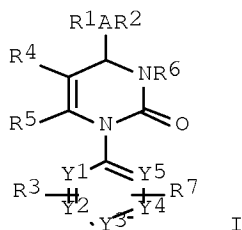
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|------|----------|-----------------|----------|
| GB 2392910 | A | 20040317 | GB 2003-15870 | 20030707 |
| CA 2498051 | A1 | 20040325 | CA 2003-2498051 | 20030828 |
| WO 2004024700 | A1 | 20040325 | WO 2003-EP9525 | 20030828 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
 PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
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 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
 FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
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 EP 1546113 A1 20050629 EP 2003-773613 20030828
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 BR 2003014186 A 20050809 BR 2003-14186 20030828
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 GB 2002-26609 A 20021114
 GB 2003-15870 A 20030707
 WO 2003-EP9525 W 20030828
 OTHER SOURCE(S): MARPAT 140:253573
 GI



AB Title compds. [I; A = aryl, heteroaryl; R1-R3 = H, OH, halo, NO2, cyano, (substituted) alkyl, alkoxy; R4 = F3CCO, (substituted) alkylcarbonyl, alkoxy carbonyl, alkenyloxycarbonyl, CO2H, arylcarbonyl, heteroaryl, heterocyclyl, cyano, etc.; R5 = (substituted) alkyl, amino; R6 = H, CHO, CONH2, (substituted) alkyl, alkoxy carbonyl, alkylsulfonylaminocarbonyl, heteroaryl, heterocyclyl, etc.; R7 = halo, NO2, cyano, OH, (substituted) alkyl, alkoxy; Y1-Y5 = CH, N, wherein the ring contains 0-2 N], were prepared Thus, 3-trifluoromethylphenylurea, 4-cyanobenzaldehyde, Et 3-oxobutyrate, and polyphosphoric acid Et ester were refluxed 18 h in THF to give 91% Et 4-(4-cyanophenyl)-6-methyl-2-oxo-1-[3- (trifluoromethyl)phenyl]-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate. The latter inhibited HNE with IC50 = 8 nM.

IT 671775-94-3P 671775-98-7P 671775-99-8P
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 671776-15-1P 671776-16-2P 671776-17-3P
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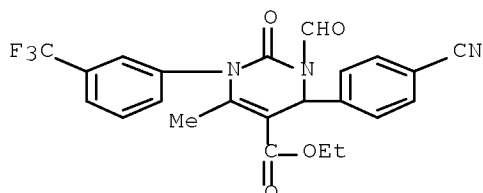
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of 2-oxopyrimidines as human leukocyte elastase inhibitors)

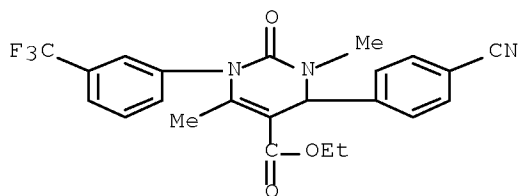
RN 671775-94-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-formyl-1,2,3,4-tetrahydro-
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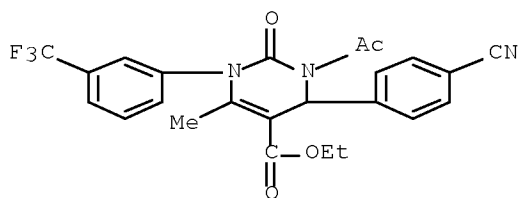
RN 671775-98-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-
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 NAME)



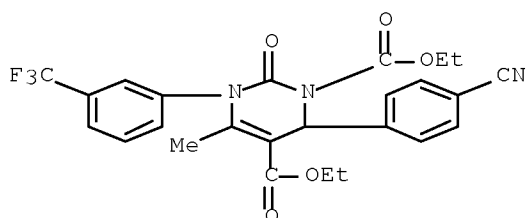
RN 671775-99-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-acetyl-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-
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 NAME)



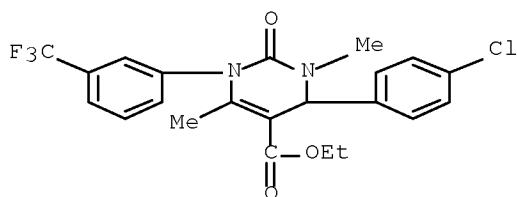
RN 671776-00-4 ZCAPLUS

CN 1,5(2H)-Pyrimidinedicarboxylic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,5-diethyl ester (CA INDEX NAME)



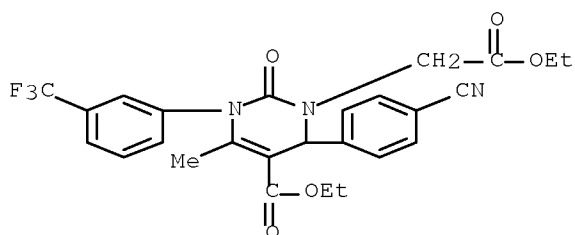
RN 671776-06-0 ZCAPLUS

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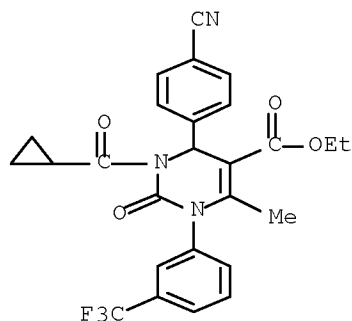
RN 671776-14-0 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



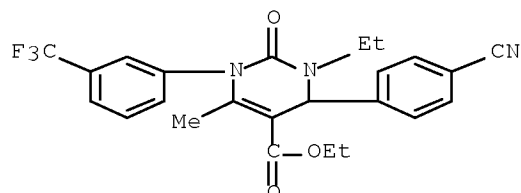
RN 671776-15-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-(cyclopropylcarbonyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



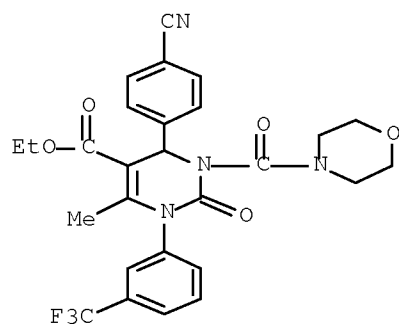
RN 671776-16-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-ethyl-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



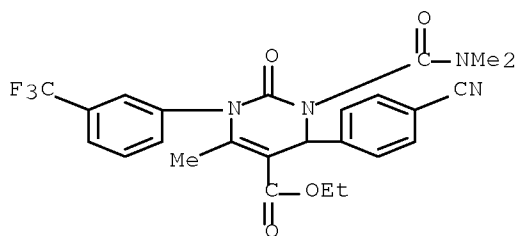
RN 671776-17-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-(4-morpholinylcarbonyl)-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

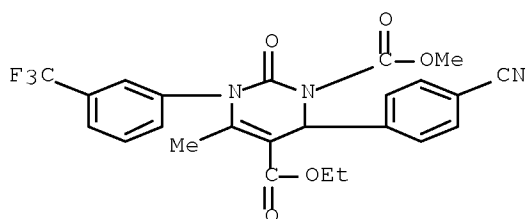


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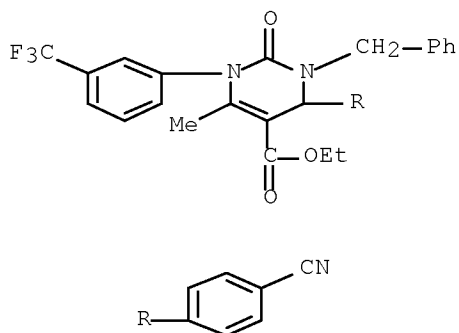
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[(dimethylamino)carbonyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



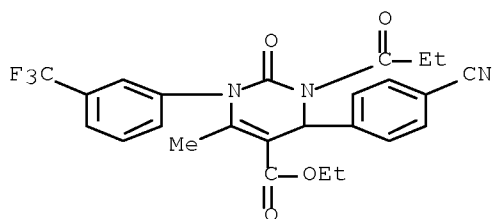
RN 671776-19-5 ZCAPLUS
CN 1,5(2H)-Pyrimidinedicarboxylic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 5-ethyl 1-methyl ester (CA INDEX NAME)



RN 671776-20-8 ZCAPLUS
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(phenylmethyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

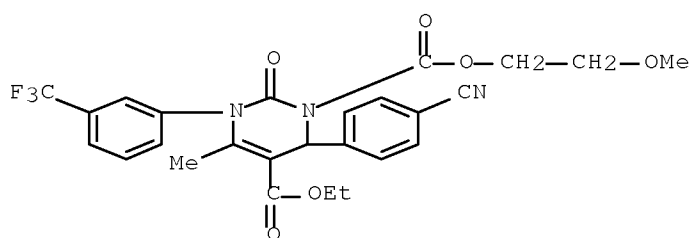


RN 671776-21-9 ZCAPLUS
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(1-oxopropyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



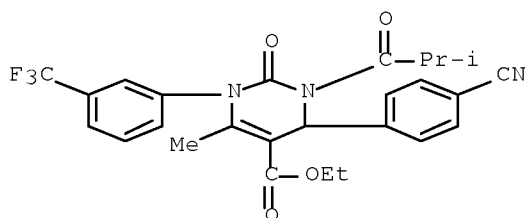
RN 671776-22-0 ZCAPLUS

CN 1,5(2H)-Pyrimidinedicarboxylic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 5-ethyl 1-(2-methoxyethyl) ester (CA INDEX NAME)



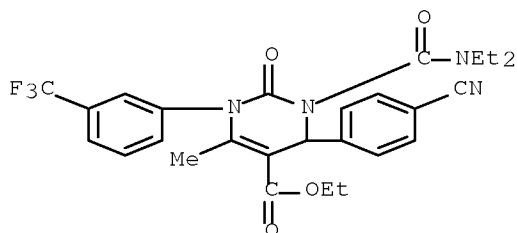
RN 671776-23-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-(2-methyl-1-oxopropyl)-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



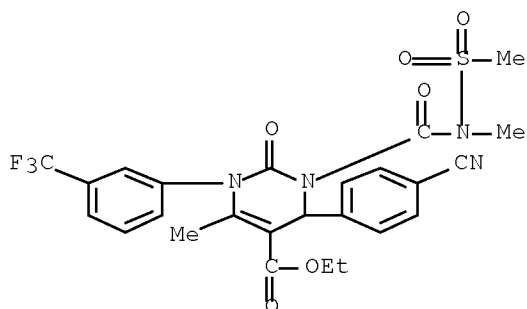
RN 671776-24-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[(diethylamino)carbonyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



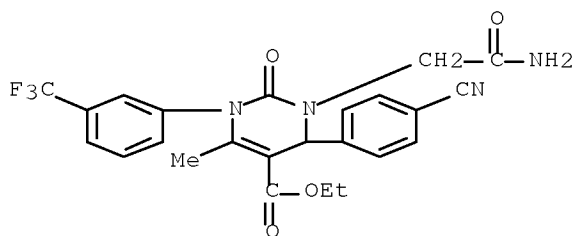
RN 671776-25-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[[methyl(methylsulfonyl)amino]carbonyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



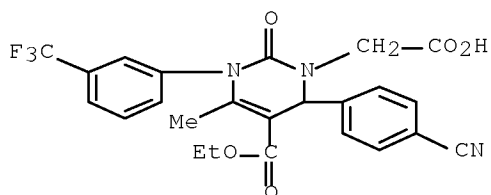
RN 671776-26-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(2-amino-2-oxoethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



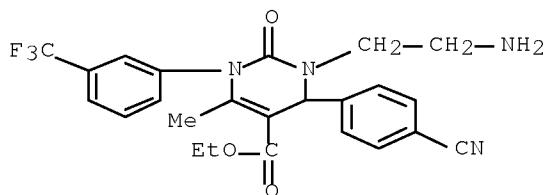
RN 671776-27-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



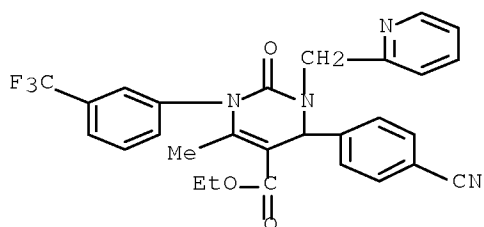
RN 671776-28-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(2-aminoethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



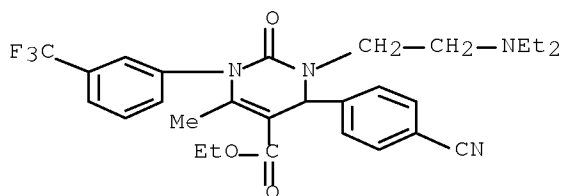
RN 671776-29-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(2-pyridinylmethyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



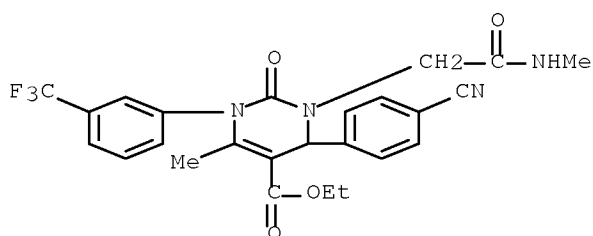
RN 671776-30-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-(diethylamino)ethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



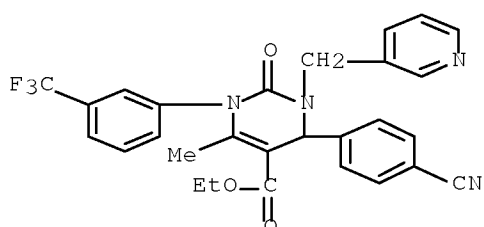
RN 671776-31-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[2-(methylamino)-2-oxoethyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



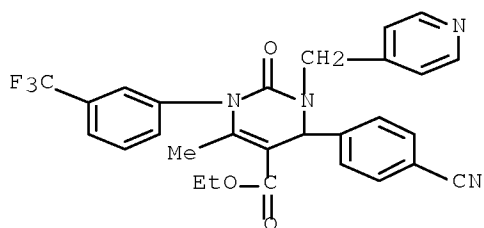
RN 671776-32-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(3-pyridinylmethyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



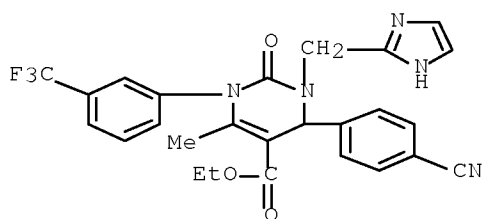
RN 671776-33-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(4-pyridinylmethyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



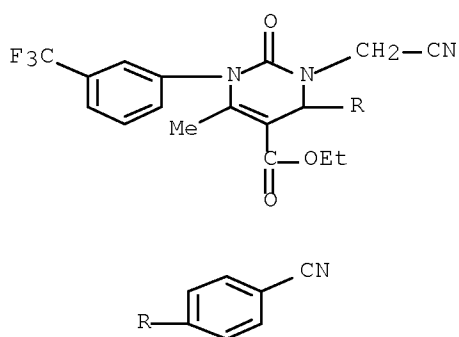
RN 671776-34-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-(1H-imidazol-2-ylmethyl)-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



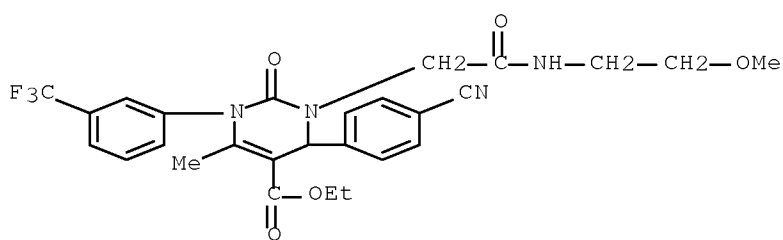
RN 671776-35-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(cyanomethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



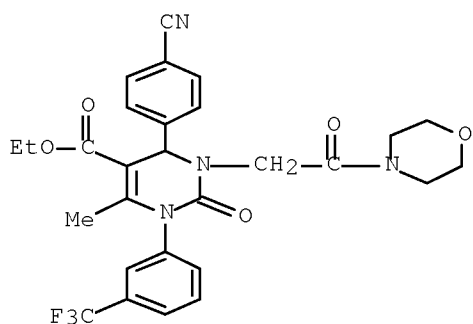
RN 671776-36-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[2-[(2-methoxyethyl)amino]-2-oxoethyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



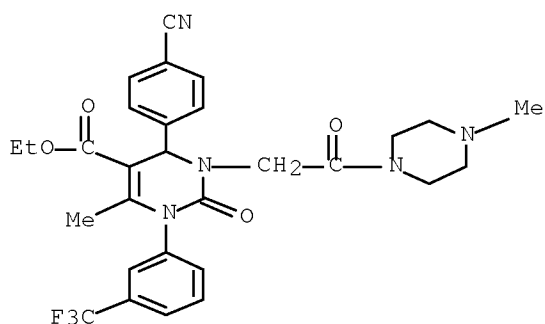
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CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[2-(4-morpholinyl)-2-oxoethyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



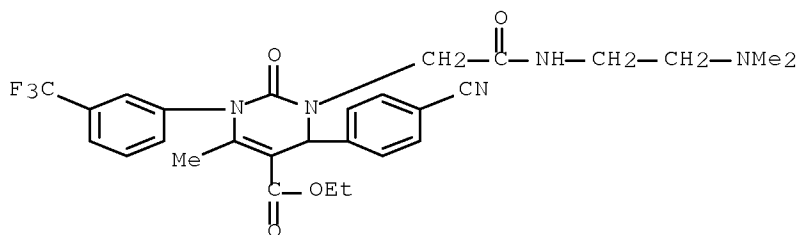
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CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[2-(4-methyl-1-piperazinyl)-2-oxoethyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



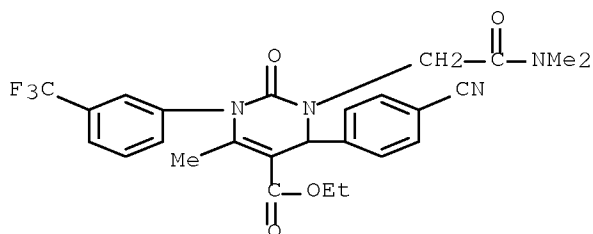
RN 671776-44-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-(dimethylamino)ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



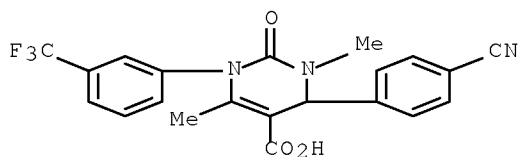
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CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-(dimethylamino)-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



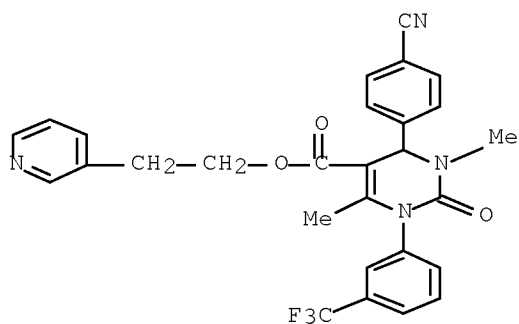
RN 671776-58-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



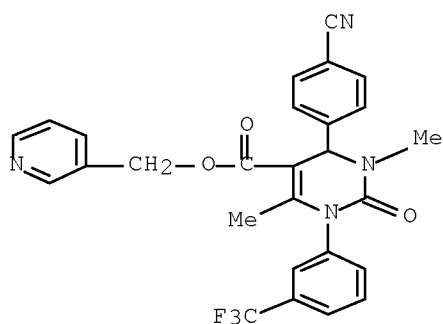
RN 671776-69-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(3-pyridinyl)ethyl ester (CA INDEX NAME)



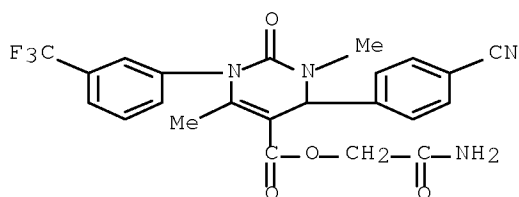
RN 671776-70-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 3-pyridinylmethyl ester (CA INDEX NAME)



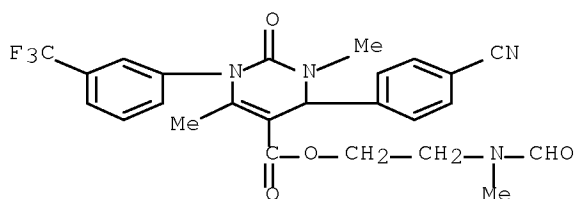
RN 671776-71-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-amino-2-oxoethyl ester (CA INDEX NAME)



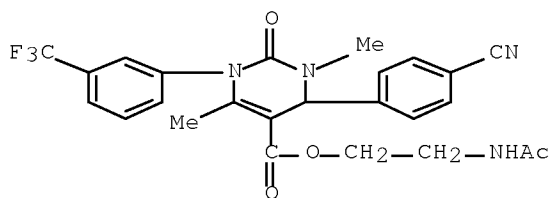
RN 671776-72-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(formylmethylamino)ethyl ester (CA INDEX NAME)



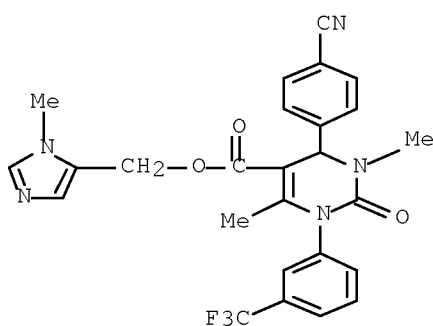
RN 671776-73-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(acetylamino)ethyl ester (CA INDEX NAME)



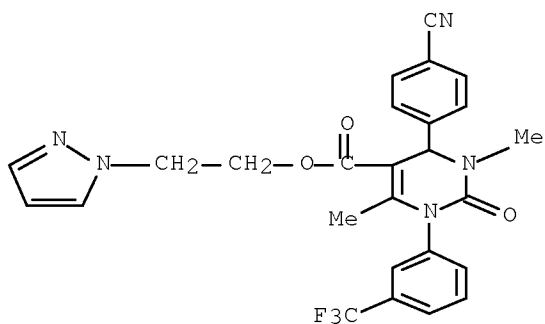
RN 671776-74-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (1-methyl-1H-imidazol-5-yl)methyl ester (CA INDEX NAME)



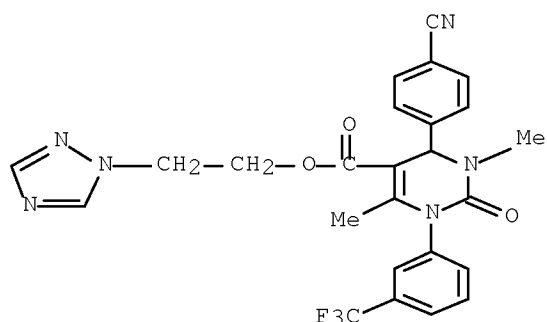
RN 671776-75-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(1H-pyrazol-1-yl)ethyl ester (CA INDEX NAME)



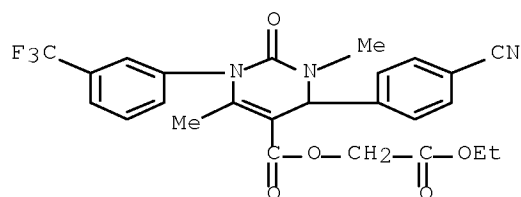
RN 671776-76-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(1H-1,2,4-triazol-1-yl)ethyl ester (CA INDEX NAME)



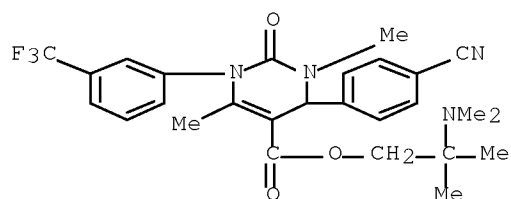
RN 671776-77-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-ethoxy-2-oxoethyl ester (CA INDEX NAME)



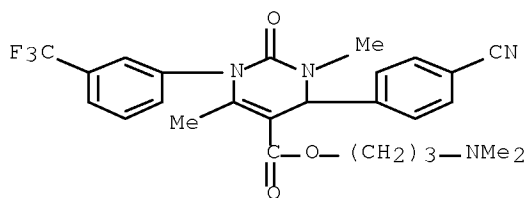
RN 671776-78-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(dimethylamino)-2-methylpropyl ester (CA INDEX NAME)



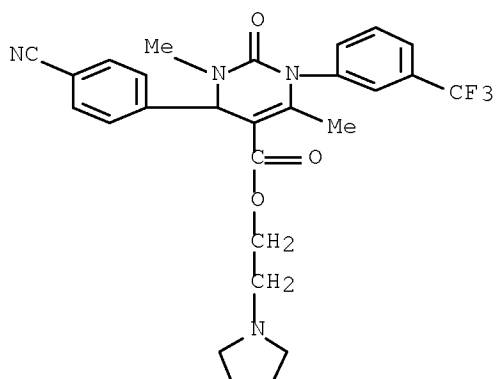
RN 671776-79-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 3-(dimethylamino)propyl ester (CA INDEX NAME)



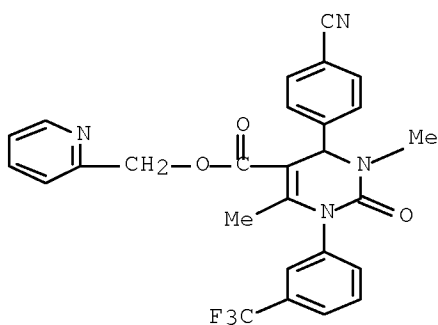
RN 671776-80-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(1-pyrrolidinyl)ethyl ester (CA INDEX NAME)



RN 671776-81-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-pyridinylmethyl ester (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN

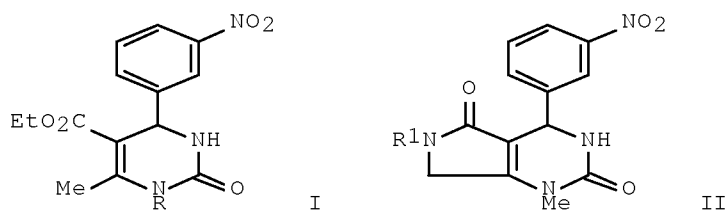
ACCESSION NUMBER: 2001:779582 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 136:183781

TITLE: Investigation of the chemical reactivity of positions

N-3, C-5 and C6-methyl group in Biginelli type compounds and synthesis of new dihydropyrimidine derivatives

AUTHOR(S): Namazi, H.; Mirzaei, Y. R.; Azamat, H.
 CORPORATE SOURCE: Lab of Carbohydrates and Biopolymers, Faculty of Chemistry, University of Tabriz, Tabriz, Iran
 SOURCE: Journal of Heterocyclic Chemistry (2001), 38(5), 1051-1054
 CODEN: JHTCAD; ISSN: 0022-152X
 PUBLISHER: HeteroCorporation
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:183781
 GI



AB Biginelli-type compds. (I; R = Me, Ph) were prepared and converted to eight N-3 substituted dihydropyrimidines using NaH and various electrophiles (ClCO₂Et, TsCl, Ac₂O, AcCl and PhCOCl). I (R = Ph) was monobrominated at the C6-Me group using bromine solution. Reaction of the bromo derivative with amino nucleophiles, such as MeNH₂ and cyclohexylamine, produced two pyrrolopyrimidine derivs. (II; R₁ = Me, cyclohexyl). The structures of all the new compds. were confirmed using FTIR, ¹H NMR, and ¹³C NMR spectral and elemental analyses.

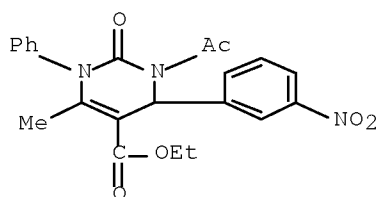
IT 398456-89-8P 398456-90-1P 398456-91-2P
 398456-96-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(chemical reactivity of positions N-3, C-5 and C6-Me group in Biginelli type compds. and synthesis of new dihydropyrimidine derivs.)

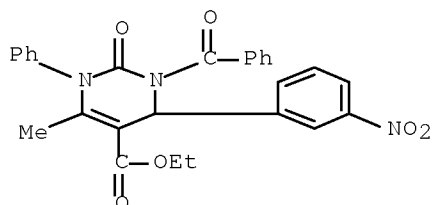
RN 398456-89-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-acetyl-1,2,3,4-tetrahydro-6-methyl-4-(3-nitrophenyl)-2-oxo-1-phenyl-, ethyl ester (CA INDEX NAME)



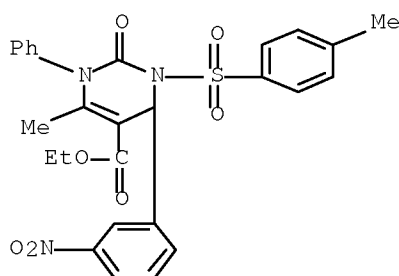
RN 398456-90-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-benzoyl-1,2,3,4-tetrahydro-6-methyl-4-(3-nitrophenyl)-2-oxo-1-phenyl-, ethyl ester (CA INDEX NAME)



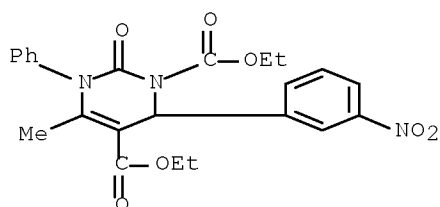
RN 398456-91-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-6-methyl-3-[(4-methylphenyl)sulfonyl]-4-(3-nitrophenyl)-2-oxo-1-phenyl-, ethyl ester (CA INDEX NAME)



RN 398456-96-7 ZCAPLUS

CN 1,5(2H)-Pyrimidinedicarboxylic acid, 3,6-dihydro-4-methyl-6-(3-nitrophenyl)-2-oxo-3-phenyl-, 1,5-diethyl ester (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:594082 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 129:269481

ORIGINAL REFERENCE NO.: 129:54755a, 54758a

TITLE: Synthesis and characterization of metal chelates with new pyrimidine derivatives

AUTHOR(S): Siddiqi, K. S.; Nishat, N.

CORPORATE SOURCE: Department of Chemistry, University of Bahrain, Isa Town, Bahrain

SOURCE: Synthesis and Reactivity in Inorganic and Metal-Organic Chemistry (1998), 28(8), 1353-1369

CODEN: SRIMCN; ISSN: 0094-5714

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

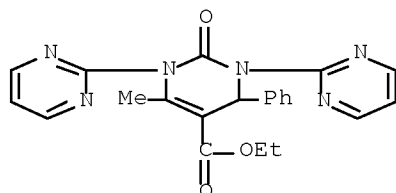
AB The ligands 4-phenyl-5-ethoxycarbonyl-6-methyl-3,4-dihydropyrimidin-2-one (L1), 1,3-diacetamido(4-phenyl-5-ethoxycarbonyl-6-methyl-3,4-dihydropyrimidin-2-one) (L2) and 1,3-dipyrimidinyl(4-phenyl-5-ethoxycarbonyl-6-methyl-3,4-dihydropyrimidin-2-one) (L3) and their metal chelates with 3d metal ions were synthesized. The conductivity measurements suggest that $[M(L1)2Cl2]$, $[M2(L2)Cl4]$, $[M'(L2)Cl6]$ and $[M(L3)2Cl2]$ are nonelectrolytes in DMSO and MeCN while $[M'(L1)2Cl2]Cl$ and $[M'(L3)2Cl2]Cl$ are 1:1 electrolytes, where $M = Mn(II)$, $Co(II)$, $Ni(II)$, $Cu(II)$ and $Zn(II)$ and $M' = Cr(III)$ and $Fe(III)$. Spectroscopic studies show that L1 coordinates through NH and the O atom of the pyrimidinyl ring, L2 coordinates through the N and O atoms of the amide group while L3 coordinates via the two N atoms of the pyrimidinone ring. The electronic spectra and the magnetic moments reveal that all metal complexes of L1, L3 and complexes of trivalent metal ions with L2 are octahedral while those of the divalent metal ions with L2 probably have a tetrahedral structure except for the $Cu(II)$ complex which appears to be square-planar. The β values suggest a considerable degree of orbital overlap in the metal-ligand bond.

IT 213592-25-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with first-row transition-metal ions)

RN 213592-25-7 ZCAPLUS

CN [2,1'(2'H):3'(4'H),2''-Terpyrimidine]-5'-carboxylic acid,
4'-methyl-2'-oxo-6'-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



IT 213592-48-4P 213592-50-8P 213592-52-0P

213592-54-2P 213592-56-4P 213592-58-6P

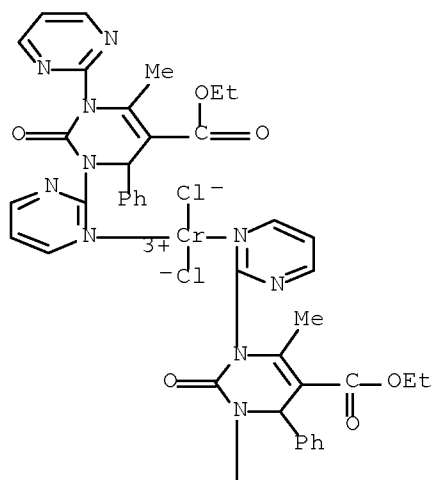
213592-60-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

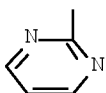
RN 213592-48-4 ZCAPLUS

CN Chromium(1+), dichlorobis[ethyl 6'-methyl-2'-oxo-4'-
phenyl[2,1'(2'H):3'(4'H),2''-terpyrimidine]-5'-carboxylate- $\kappa N1$]-,
chloride, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A

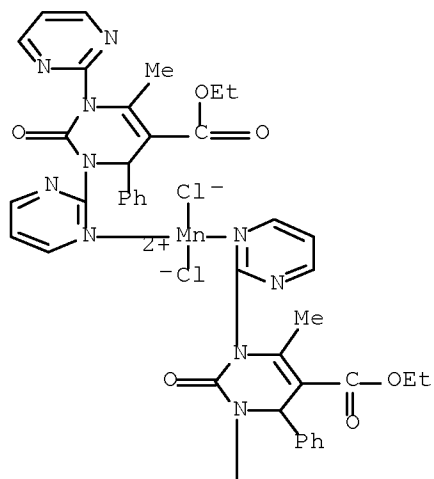


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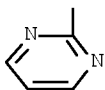


RN 213592-50-8 ZCAPLUS
 CN Manganese, dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2''-terpyrimidine]-5'-carboxylate-κN1]-(9Cl) (CA INDEX NAME)

PAGE 1-A

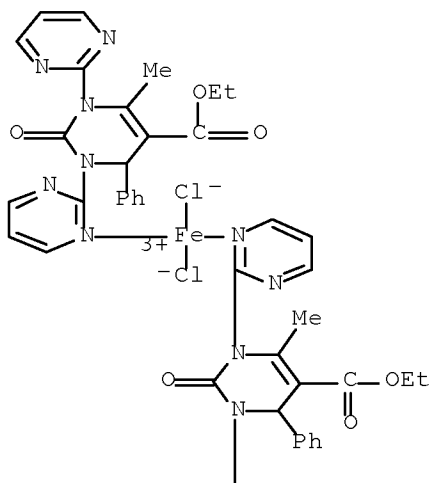


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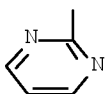


RN 213592-52-0 ZCAPLUS
 CN Iron(1+), dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2''-terpyrimidine]-5'-carboxylate-κN1]-, chloride (9CI) (CA INDEX NAME)

PAGE 1-A

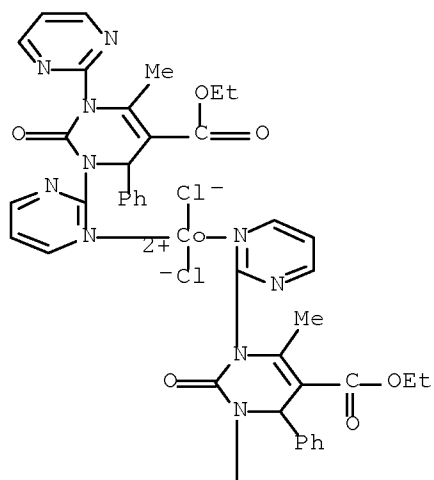


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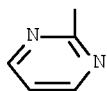


RN 213592-54-2 ZCAPLUS
 CN Cobalt, dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2''-terpyrimidine]-5'-carboxylate-κN1]-, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A

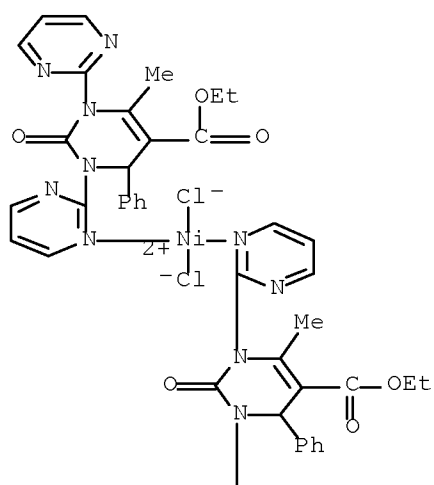


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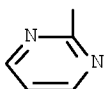


RN 213592-56-4 ZCAPLUS
 CN Nickel, dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2''-terpyrimidine]-5'-carboxylate-κN1]- (9CI) (CA INDEX NAME)

PAGE 1-A

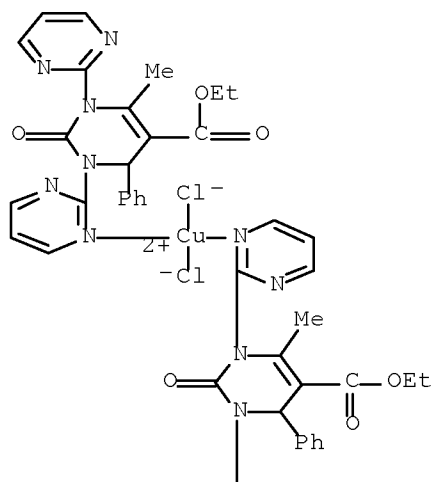


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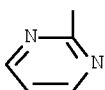


RN 213592-58-6 ZCAPLUS
 CN Copper, dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2''-terpyrimidine]-5'-carboxylate-κN1]- (9CI) (CA INDEX NAME)

PAGE 1-A

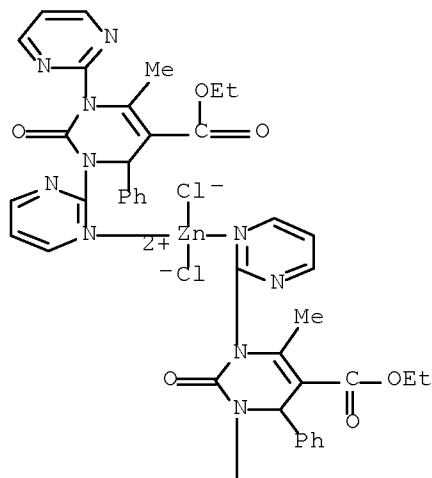


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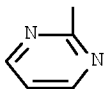


RN 213592-60-0 ZCAPLUS
 CN Zinc, dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2''-terpyrimidine]-5'-carboxylate-κN1]-, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A

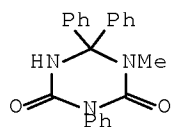


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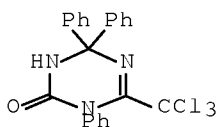


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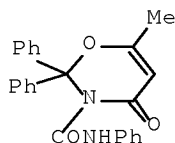
L6 ANSWER 11 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1976:592595 ZCAPLUS Full-text
 DOCUMENT NUMBER: 85:192595
 ORIGINAL REFERENCE NO.: 85:30799a,30802a
 TITLE: Formation of heterocyclic compounds by use of
 N'-diphenylmethylene-N-phenyl-N-trimethylsilylurea
 AUTHOR(S): Matsuda, Isamu; Yamamoto, Sakae; Ishii, Yoshio
 CORPORATE SOURCE: Fac. Eng., Nagoya Univ., Nagoya, Japan
 SOURCE: Journal of the Chemical Society, Perkin Transactions
 1: Organic and Bio-Organic Chemistry (1972-1999)
 (1976), (14), 1523-8
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



II



III



IV

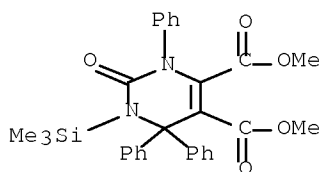
AB The reactions of the title urea (I) with acceptor mols. were studied. With cyclohexyl isocyanide, MeNCO, MeO2CC.tplbond.CCO2Me, or Cl3CCN followed by desilylation I underwent [4+1] or [4+2] cycloaddn.; imidazolidinone, triazinone, and pyrimidinone derivs. were formed. E.g., I with MeNCO gave the triazinone II. I reacted with RCN (R = CCl3, NMe2) to give the triazinone III and Ph2C:NC(NMe2):NPh, resp., by decomposition of the intermediate silyloxytriphenyltriazine with MeOH or under the reaction conditions, resp. Reaction of I with RR1CO (RR1 = Ph2C; R = H, R1 = CCl3) gave the insertion products Ph2C:NCONPhCRR1OSiMe3. Diketene reacted with I to give the oxazinone IV.

IT 61032-91-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and desilylation of)

RN 61032-91-5 ZCAPLUS

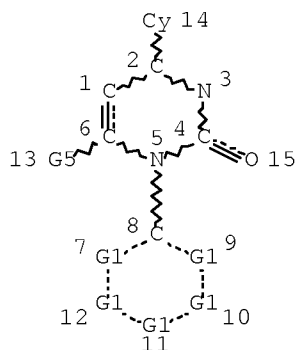
CN 4,5-Pyrimidinedicarboxylic acid, 1,2,3,6-tetrahydro-2-oxo-3,6,6-triphenyl-1-(trimethylsilyl)-, dimethyl ester (9CI) (CA INDEX NAME)



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SEARCH HISTORY

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VAR G5=C/NH2
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CONNECT IS E3 RC AT 3
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GGCAT IS UNS AT 14
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
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100.0% PROCESSED 94555 ITERATIONS
SEARCH TIME: 00.00.04

397 ANSWERS

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FILE 'ZCAPLUS' ENTERED AT 12:34:50 ON 22 SEP 2008

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L5 397 SEA SSS FUL L1
SAVE TEMP L5 JAI786FULL/A

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L6 11 SEA ABB=ON L5

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D STAT QUE L5

FILE 'ZCAPLUS' ENTERED AT 12:36:45 ON 22 SEP 2008
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FILE 'HOME' ENTERED AT 12:37:08 ON 22 SEP 2008
D STAT QUE L5

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